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Supporting Information

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Thieme

Base-induced Cyclisation of *ortho*-Substituted 2-Phenyloxazolines to Give 3-Aminobenzofurans and Related Heterocycles

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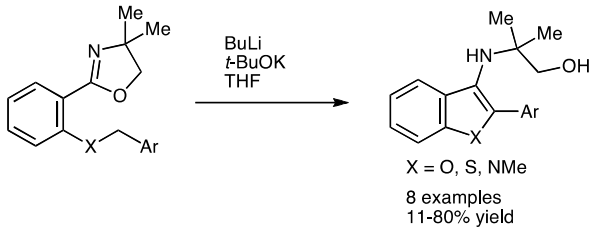
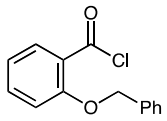


Supporting Information

General Experimental Details

^{1}H, ^{13}C and ^{19}F NMR spectra were recorded in $CDCl_3$ unless otherwise stated with internal TMS as reference for H and C and external $CFCl_3$ as refernce for F. IR spectra were recorded using the ATR technique. HRMS measurements were made either using ES or ASAP ionization both with TOF analyzer or NSI with an ion-trap analyzer.

Additonal structures not shown in the paper



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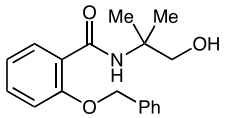

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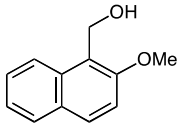

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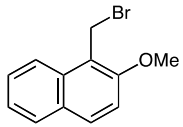

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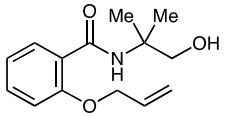

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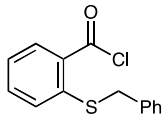

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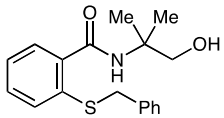

G

2-(Benzyloxy)benzoyl chloride A

A solution of 2-(benzyloxy)benzoic acid[1] (10.00 g, 43.8 mmol) and thionyl chloride (6.4 mL, 10.44 g, 87.7 mmol) in toluene (90 mL) was heated under reflux for 3 h and then cooled and evaporated to give **A** (10.80 g, 100%) as a pale yellow oil which was used without further purification. IR: 3032, 1780, 1599, 1448, 1290, 1024, 868, 759 cm^{-1}. ^{1}H NMR (400 MHz): δ = 8.09 (dd, *J* = 7.8, 1.8 Hz, 1 H), 7.53 (ddd, *J* = 8.4, 7.4, 1.8 Hz, 1 H), 7.49–7.46 (m, 2 H), 7.40–7.35 (m, 2 H), 7.33–7.29 (m, 1 H), 7.06–7.02 (m, 2 H), 5.19 (s, 2 H, CH_2). ^{13}C NMR (100 MHz): δ = 163.8 (C=O), 158.5 (C–O), 136.0 (CH), 135.8 (C), 134.5 (CH), 128.6 (2 CH), 128.0 (CH), 126.7 (2 CH), 122.8 (C), 120.6 (CH), 113.5 (CH), 70.5 (CH_2). HRMS (ESI^+): *m/z* calcd for $C_{14}H_{11}O_2$ $[M–Cl]^+$: 211.0754; found: 211.0751. The ^{1}H NMR spectral data was in accordance with that previously reported.[2]

2-(Benzyloxy)-*N*-(1-hydroxy-2-methylpropan-2-yl)benzamide B

A solution of 2-(benzyloxy)benzoyl chloride **A** (10.80 g, 43.8 mmol) in CH_2Cl_2 (40 mL) was added dropwise to a solution of 2-amino-2-methylpropan-1-ol (7.81 g, 87.6 mmol) in CH_2Cl_2 (50 mL) stirred at 0 °C. Once the addition was complete, the reaction mixture was allowed to warm to rt for 18 h before being poured into water. The two layers were separated and the aqueous layer was re-extracted with CH_2Cl_2 (× 2). The combined organic layers were washed successively with 2 M HCl, 2 M NaOH and water before being dried and evaporated to give **B** (12.68 g, 97%) as a colourless solid, mp 115–117 °C, which was used without further purification. IR: 3446, 3366, 1645, 1557, 1102, 1069, 997, 919, 857, 751, 699 cm^{-1}. ^{1}H NMR (500 MHz): δ = 8.20 (dd, *J* = 7.8, 1.8 Hz, 1 H), 8.11 (br s, 1 H, NH), 7.50–7.40 (m, 6 H), 7.12 (t, *J* = 7.5 Hz, 1 H), 7.09 (d, *J* = 8.0 Hz, 1 H), 5.32 (t, *J* = 5.5 Hz, 1 H, OH), 5.13 (s, 2 H, OCH_2Ph), 3.54 (d, *J* = 5.5 Hz, 2 H, C***H***$_2$OH), 1.04 (s, 6 H, CH_3). ^{13}C NMR

(125 MHz): δ = 165.6 (C=O), 156.7 (C–O), 135.1 (C), 133.0 (CH), 132.2 (CH), 129.1 (CH), 128.9 (2 CH), 128.8 (2 CH), 121.6 (CH), 121.5 (C), 112.3 (CH), 71.6 (CH_2), 71.1 (CH_2), 56.1 (C), 24.5 (CH_3). HRMS (ESI^+): *m/z* calcd for $C_{18}H_{21}NO_3Na$ $[M+Na]^+$: 322.1414; found: 322.1407.

2-(2-(Benzyloxy)phenyl)-4,4-dimethyl-4,5-dihydrooxazole 1

Thionyl chloride (3.7 mL, 6.03 g, 50.7 mmol) was added to a solution of 2-(benzyloxy)-*N*-(1-hydroxy-2-methylpropan-2-yl)benzamide **B** (12.68 g, 42.4 mmol) in CH_2Cl_2 (210 mL) and the reaction mixture was stirred at rt for 18 h. The mixture was washed with 2 M NaOH and water before being dried and evaporated to give, after purification by Kugelrohr distillation (185 °C/9.2 Torr), **1** (10.14 g, 85%) as a colourless oil which formed a low-melting solid on standing. IR: 1718, 1645, 1038, 967, 871, 848, 751, 733, 695 cm^{-1}. ^1H NMR (500 MHz): δ = 7.72 (dd, *J* = 7.5, 2.0 Hz, 1 H), 7.52 (d, *J* = 7.5 Hz, 2 H), 7.38–7.35 (m, 3 H), 7.29 (t, *J* = 7.3 Hz, 1 H), 7.01–6.97 (m, 2 H), 5.18 (s, 2 H, OCH_2Ar), 4.11 (s, 2 H, oxazoline CH_2), 1.41 (s, 6 H, CH_3). ^{13}C NMR (125 MHz): δ = 161.2 (C=N), 157.3 (C–O), 137.0 (C), 131.9 (CH), 131.1 (CH), 128.2 (2 CH), 127.5 (CH), 126.7 (2 CH), 120.6 (CH), 118.6 (C), 113.5 (CH), 78.8 (oxazoline CH_2), 70.5 (OCH_2Ar), 67.5 (C), 28.4 (CH_3). HRMS (ESI^+): *m/z* calcd for $C_{18}H_{20}NO_2$ $[M+H]^+$: 282.1489; found: 282.1478.

2-Methyl-2-((2-phenylbenzofuran-3-yl)amino)propan-1-ol 3

Under a nitrogen atmosphere, *n*-butyllithium (2.5 M in hexane, 6.6 mL, 16.5 mmol) was added to a stirred mixture of 2-(2-(benzyloxy)phenyl)-4,4-dimethyl-4,5-dihydrooxazole **1** (1.41 g, 5.01 mmol) and potassium *tert*-butoxide (1.88 g, 16.8 mmol) in dry THF (50 mL). The reaction mixture was stirred at rt for 2 h before being quenched by addition of sat. aq. NH_4Cl and extracted with Et_2O (× 3). The combined organic layers were dried and evaporated to give, after purification by column chromatography (Al_2O_3, gradient elution, Et_2O/hexane 3:2 to EtOAc), **2** (1.13 g, 80%) as orange crystals, mp 59–63 °C. IR: 3325, 2974, 2933, 1605, 1452, 1362, 1256, 1043, 1026, 739, 694 cm^{-1}. ^1H NMR (400 MHz): δ = 8.08–8.05 (m, 2 H), 7.64–7.62 (m, 1 H), 7.46–7.41 (m, 3 H), 7.34–7.30 (m, 1 H), 7.29–7.25 (m, 1 H), 7.24–7.20 (m, 1 H), 3.42 (s, 2 H, CH_2), 2.65 (br s, 2 H, NH and OH), 1.07 (s, 6 H, CH_3). ^{13}C NMR (125 MHz): δ = 153.0 (C), 148.5 (C), 131.1 (C), 129.5 (C), 128.5 (2 CH), 128.0 (CH), 126.5 (2 CH), 124.4 (CH), 122.5 (CH), 122.2 (C), 119.6 (CH), 111.2 (CH), 70.3 (CH_2), 58.1 (C), 24.7 (CH_3). HRMS (ESI^+): *m/z* calcd for $C_{18}H_{20}NO_2$ $[M+H]^+$: 282.1489; found: 282.1482.

2-(2-((4-Fluorobenzyl)oxy)phenyl)-4,4-dimethyl-4,5-dihydrooxazole 5a

2-(4,4-Dimethyl-4,5-dihydrooxazol-2-yl)phenol **4** (0.96 g, 5.02 mmol) was added to a stirred suspension of sodium hydride (60% in mineral oil, pre-washed with hexane, 0.21 g, 5.25 mmol) in DMF (10 mL) and the mixture was stirred at rt for 15 min before 4-fluorobenzyl chloride (0.6 mL, 0.72 g, 5.01 mmol) was added. After stirring for 18 h at rt, the reaction mixture was poured into water and extracted with CH_2Cl_2 followed by Et_2O (× 3). The combined organic layers were washed with brine (× 5) and 2 M NaOH before being dried and evaporated to give, after purification by column chromatography (SiO_2, Et_2O/hexane 3:2), at R_f 0.45, and subsequent recrystallisation (EtOAc/hexane), **5a** (0.68 g, 45%) as colourless crystals, mp 72–76 °C. IR: 2966, 1639, 1498, 1445, 1294, 1259, 1159, 1037, 829, 815, 749, 688 cm^{-1}. ^1H NMR (400 MHz): δ = 7.74–7.71 (m, 1 H), 7.53–7.48 (m, 2 H), 7.41–7.36 (m, 1 H), 7.08–7.02 (m, 2 H), 7.02–6.96 (m, 2 H), 5.12 (s, 2 H, OCH_2Ar), 4.08 (s, 2 H,

oxazoline CH_2), 1.40 (s, 6 H, CH_3). ^{13}C NMR (125 MHz): δ = 162.2 (d, J_{CF} = 244 Hz, CF), 161.0 (C), 157.1 (C), 132.8 (d, J_{CF} = 3.1 Hz, C), 131.9 (CH), 131.2 (CH), 128.5 (d, J_{CF} = 8.0 Hz, 2 CH), 120.8 (CH), 118.6 (C), 115.1 (d, J_{CF} = 21.3 Hz, 2 CH), 113.6 (CH), 78.8 (oxazoline CH_2), 69.9 (OCH_2Ar), 67.6 (C), 28.4 (CH_3). ^{19}F NMR (376 MHz): δ = –115.0. HRMS (NSI^+): *m/z* calcd for $C_{18}H_{19}FNO_2$ $[M+H]^+$: 300.1394; found: 300.1396.

2-(2-((4-Methoxybenzyl)oxy)phenyl)-4,4-dimethyl-4,5-dihydrooxazole 5b

The same procedure as for **5a** using 2-(4,4-dimethyl-4,5-dihydrooxazol-2-yl)phenol **4** (0.57 g, 2.98 mmol), sodium hydride (0.12 g, 3.00 mmol) and 4-methoxybenzyl bromide (0.60 g, 2.98 mmol) in DMF (10 mL) gave, after purification by Kugelrohr distillation (220 °C/8.0 Torr), **5b** (0.79 g, 85%) as a pale yellow oil which partially crystallised on standing. IR: 2968, 1636, 1558, 1516, 1244, 1175, 1036, 989, 868, 814, 766 cm^{-1}. ^{1}H NMR (500 MHz): δ = 7.70 (dd, *J* = 7.5, 1.5 Hz, 1 H), 7.41 (d, *J* = 8.8 Hz, 2 H), 7.38–7.34 (m, 1 H), 6.99–6.95 (m, 2 H), 6.89 (d, *J* = 8.8 Hz, 2 H), 5.09 (s, 2 H, OCH_2Ar), 4.08 (s, 2 H, oxazoline CH_2), 3.80 (s, 3 H, OCH_3), 1.39 (s, 6 H, oxazoline CH_3). ^{13}C NMR (125 MHz): δ = 161.3 (C), 159.0 (C), 157.3 (C), 131.8 (CH), 131.1 (CH), 129.1 (C), 128.3 (2 CH), 120.6 (CH), 118.7 (C), 113.8 (CH), 113.6 (2 CH), 78.9 (oxazoline CH_2), 70.4 (OCH_2Ar), 67.4 (C), 55.2 (OCH_3), 28.4 (CH_3). HRMS (NSI^+): *m/z* calcd for $C_{19}H_{21}NO_3Na$ $[M+Na]^+$: 334.1414; found: 334.1416.

2-(2-((3-Methoxybenzyl)oxy)phenyl)-4,4-dimethyl-4,5-dihydrooxazole 5c

The same procedure as for **5a** using 2-(4,4-dimethyl-4,5-dihydrooxazol-2-yl)phenol **4** (0.57 g, 2.98 mmol), sodium hydride (0.12 g, 3.00 mmol) and 3-methoxybenzyl bromide[3] (0.60 g, 2.98 mmol) in DMF (10 mL) gave, after purification by kugelrohr distillation (220 °C/8.0 Torr), **5c** (0.80 g, 86%) as a yellow oil. IR: 2970, 2901, 1641, 1599, 1491, 1452, 1261, 1051, 756, 692 cm^{-1}. ^{1}H NMR (500 MHz): δ = 7.73 (dd, *J* = 7.8, 1.8 Hz, 1 H), 7.38–7.34 (m, 1 H), 7.26 (t, *J* = 7.8 Hz, 1 H), 7.11–7.09 (m, 1 H), 7.08–7.05 (m, 1 H), 6.99–6.96 (m, 2 H), 6.82 (dd, *J* = 8.0, 2.0 Hz, 1 H), 5.13 (s, 2 H, OCH_2Ar), 4.10 (s, 2 H, oxazoline CH_2), 3.80 (s, 3 H, OCH_3), 1.40 (s, 6 H, oxazoline CH_3). ^{13}C NMR (125 MHz): δ = 161.3 (C), 159.7 (C), 157.2 (C), 138.6 (C), 131.9 (CH), 131.2 (CH), 129.3 (CH), 120.6 (CH), 118.9 (CH), 118.4 (C), 113.5 (CH), 113.0 (CH), 112.2 (CH), 78.9 (oxazoline CH_2), 70.2 (OCH_2Ar), 67.4 (C), 55.1 (OCH_3), 28.3 (CH_3). HRMS (NSI^+): *m/z* calcd for $C_{19}H_{22}NO_3$ $[M+H]^+$: 312.1594; found: 312.1586.

2-(2-((2-Methoxybenzyl)oxy)phenyl)-4,4-dimethyl-4,5-dihydrooxazole 5d

The same procedure as for **5a** using 2-(4,4-dimethyl-4,5-dihydrooxazol-2-yl)phenol **4** (0.57 g, 2.98 mmol), sodium hydride (0.12 g, 3.00 mmol) and 2-methoxybenzyl bromide[4] (0.60 g, 2.98 mmol) in DMF (10 mL) gave, after purification by kugelrohr distillation (215 °C/20 Torr), **5d** (0.64 g, 69%) as an orange oil. IR: 2961, 2926, 1641, 1601, 1494, 1452, 1362, 1246, 1034, 756 cm^{-1}. ^{1}H NMR (500 MHz): δ = 7.81–7.79 (m, 1 H), 7.73 (dd, *J* = 7.5, 2.0 Hz, 1 H), 7.39–7.36 (m, 1 H), 7.28–7.24 (m, 1 H), 7.05 (d, *J* = 8.0 Hz, 1 H), 6.98–6.95 (m, 2 H), 6.86 (d, *J* = 8.5 Hz, 1 H), 5.20 (s, 2 H, OCH_2Ar), 4.11 (s, 2 H, oxazoline CH_2), 3.84 (s, 3 H, OCH_3), 1.42 (s, 6 H, oxazoline CH_3). ^{13}C NMR (125 MHz): δ = 161.2 (C),

157.5 (C), 156.0 (C), 132.0 (CH), 131.0 (CH), 128.1 (CH), 127.6 (CH), 125.6 (C), 120.4 (CH), 120.3 (CH), 118.2 (C), 113.3 (CH), 109.6 (CH), 78.8 (oxazoline CH_2), 67.5 (C), 65.6 (OCH_2Ar), 55.2 (OCH_3), 28.5 (CH_3). HRMS (NSI^+): *m/z* calcd for $C_{19}H_{21}NO_3Na$ $[M+Na]^+$: 334.1414; found: 334.1412.

(2-Methoxynaphthalen-1-yl)methanol C

Following a literature procedure,[5] sodium borohydride (0.53 g, 14.0 mmol) was added in small portions to a stirred 0 °C solution of 2-methoxy-1-naphthaldehyde (5.03 g, 27.0 mmol) in THF (135 mL). Once the addition was complete, the reaction mixture was allowed to warm to rt overnight. Water (135 mL) was added and the mixture was extracted with Et_2O (2 × 150 mL). The combined organic layers were washed with brine (2 × 150 mL) before being dried and evaporated. The crude residue was recrystallised (EtOAc/hexane) to give **C** (4.59 g, 90%) as colourless crystals, mp 100–102 °C (lit.[6] 100–101 °C). IR: 3326, 2968, 1626, 1594, 1512, 1472, 1249, 1156, 1085, 1059, 984, 803, 741 cm^{-1}. ^1H NMR (500 MHz): δ = 8.08 (d, *J* = 8.5 Hz, 1 H), 7.80 (d, *J* = 9.0 Hz, 1 H), 7.77 (d, *J* = 8.5 Hz, 1 H), 7.51–7.48 (m, 1 H), 7.36–7.33 (m, 1 H), 7.24 (d, *J* = 9.0 Hz, 1 H), 5.14 (s, 2 H, CH_2), 3.93 (s, 3 H, CH_3), 2.19 (br s, 1 H, OH). ^{13}C NMR (125 MHz): δ = 155.0 (C–O), 132.7 (C)), 130.0 (CH), 129.0 (C), 128.4 (CH), 126.9 (CH), 123.5 (CH), 122.9 (CH), 121.1 (C), 112.9 (CH), 56.4 (CH_3), 55.7 (CH_2).

1-(Bromomethyl)-2-methoxynaphthalene D

Following a literature procedure,[7] phosphorus tribromide (0.75 mL, 2.16 g, 7.98 mmol) was added dropwise to a stirred 0 °C suspension of (2-methoxynaphthalen-1-yl)methanol **C** (4.01 g, 21.3 mmol) in dry Et_2O (60 mL). After stirring at 0 °C for 30 min, the reaction mixture was diluted with CH_2Cl_2 (100 mL) and washed with water (2 × 50 mL), sat. aq. $NaHCO_3$ (50 mL) and water (50 mL) before being dried and evaporated. The crude residue was recrystallised (EtOAc/hexane) to give **D** (4.75 g, 89%) as pale yellow crystals, mp 127–130 °C (lit.[7] 126–129 °C). IR: 3012, 2839, 1623, 1592, 1515, 1255, 1205, 1159, 1082, 1050, 812, 746 cm^{-1}. ^1H NMR (500 MHz): δ = 8.01 (d, *J* = 8.5 Hz, 1 H), 7.83 (d, *J* = 9.3 Hz, 1 H), 7.80 (d, *J* = 8.5 Hz, 1 H), 7.60–7.57 (m, 1 H), 7.39–7.36 (m, 1 H), 7.23 (d, *J* = 9.3 Hz, 1 H), 5.09 (s, 2 H, CH_2), 4.00 (s, 3 H, CH_3). ^{13}C NMR (125 MHz): δ = 155.1 (C–O), 132.2 (C), 131.0 (CH), 129.0 (C), 128.6 (CH), 127.2 (CH), 123.8 (CH), 122.6 (CH), 118.0 (C), 112.9 (CH), 56.5 (CH_3), 25.3 (CH_2).

2-(2-((2-Methoxynaphthalen-1-yl)methoxy)phenyl)-4,4-dimethyl-4,5-dihydrooxazole 5e

The same procedure as for **5a** using 2-(4,4-dimethyl-4,5-dihydrooxazol-2-yl)phenol **4** (0.57 g, 2.98 mmol), sodium hydride (0.12 g, 3.00 mmol) and 1-(bromomethyl)-2-methoxynaphthalene **D** (0.75 g, 2.99 mmol) in DMF (10 mL) gave, after purification by column chromatography (SiO_2, Et_2O/hexane 1:1), at R_f 0.30, **5e** (0.77 g, 71%) as a colourless solid, mp 102–105 °C. IR: 2972, 1627, 1598, 1449, 1252, 1237, 1095, 1042, 987, 806, 751, 692 cm^{-1}. ^1H NMR (500 MHz): δ = 8.29 (d, *J* = 9.0 Hz, 1 H), 7.78 (d, *J* = 9.0 Hz, 1 H), 7.73 (d, *J* = 8.5 Hz, 1 H), 7.63 (dd, *J* = 7.5, 2.0 Hz, 1 H), 7.48–7.44 (m, 1 H), 7.36–7.28 (m, 3 H), 7.21 (d, *J* = 9.5 Hz, 1 H), 6.93–6.89 (m, 1 H), 5.69 (s, 2 H, OCH_2Ar), 3.93 (s, 3 H, OCH_3), 3.89 (s, 2 H, oxazoline CH_2), 1.27 (s, 6 H, oxazoline CH_3). ^{13}C NMR (125 MHz): δ = 161.5 (C), 157.3 (C), 155.0 (C), 133.7 (C), 131.6 (CH),

130.9 (CH), 130.6 (CH), 129.0 (C), 127.9 (CH), 126.6 (CH), 124.6 (CH), 123.5 (CH), 120.5 (CH), 118.9 (C), 117.0 (C), 114.6 (CH), 112.9 (CH), 78.7 (oxazoline CH_2), 67.1 (C), 62.0 (OCH_2Ar), 56.5 (OCH_3), 28.2 (CH_3). HRMS (NSI^+): *m/z* calcd for $C_{23}H_{23}NO_3Na$ $[M+Na]^+$: 384.1570; found: 384.1568.

4,4-Dimethyl-2-(2-((4-methylbenzyl)oxy)phenyl)-4,5-dihydrooxazole 5f

The same procedure as for **5a** using 2-(4,4-dimethyl-4,5-dihydrooxazol-2-yl)phenol **4** (0.58 g, 3.03 mmol), sodium hydride (0.12 g, 3.00 mmol) and 4-methylbenzyl chloride (0.4 mL, 0.42 g, 3.02 mmol) in DMF (10 mL) gave, after purification by column chromatography (SiO_2, Et_2O/hexane 1:1), at R_f 0.45, **5f** (0.38 g, 43%) as pale yellow crystals, mp 96–100 °C. IR: 2967, 2926, 1640, 1498, 1445, 1260, 1036, 804, 748, 689 cm^{-1}. ^1H NMR (500 MHz): δ = 7.71 (dd, *J* = 7.5, 1.5 Hz, 1 H), 7.39 (d, *J* = 7.8 Hz, 2 H) 7.39–7.35 (m, 1 H), 7.17 (d, *J* = 7.8 Hz, 2 H), 7.00–6.96 (m, 2 H), 5.13 (s, 2 H, OCH_2Ar), 4.10 (s, 2 H, oxazoline CH_2), 2.35 (s, 3 H, $ArCCH_3$), 1.40 (s, 6 H, oxazoline CH_3). ^{13}C NMR (125 MHz): δ = 161.3 (C), 157.4 (C), 137.1 (C), 134.0 (C), 131.9 (CH), 131.1 (CH), 129.0 (2 CH), 126.8 (2 CH), 120.6 (CH), 118.7 (C), 113.7 (CH), 78.9 (oxazoline CH_2), 70.5 (OCH_2Ar), 67.5 (C), 28.4 (oxazoline CH_3), 21.2 ($ArCH_3$). HRMS (NSI^+): *m/z* calcd for $C_{19}H_{22}NO_2$ $[M+H]^+$: 296.1645; found: 296.1646.

4,4-Dimethyl-2-(2-((2-methylbenzyl)oxy)phenyl)-4,5-dihydrooxazole 5g

The same procedure as for **5a** using 2-(4,4-dimethyl-4,5-dihydrooxazol-2-yl)phenol **4** (0.57 g, 2.98 mmol), sodium hydride (0.12 g, 3.00 mmol) and 2-methylbenzyl bromide (0.4 mL, 0.55 g, 2.98 mmol) in DMF (10 mL) gave, after purification by Kugelrohr distillation (225 °C/20 Torr), **5g** (0.71 g, 81%) as a pale yellow oil. IR: 2967, 2926, 1640, 1499, 1445, 1260, 1036, 804, 748, 689 cm^{-1}. ^1H NMR (500 MHz): δ = 7.72 (dd, *J* = 7.8, 1.8 Hz, 1 H), 7.66–7.64 (m, 1 H), 7.40–7.36 (m, 1 H), 7.21–7.19 (m, 2 H), 7.18–7.15 (m, 1 H), 7.02 (d, *J* = 8.5 Hz, 1 H), 6.99–6.96 (m, 1 H), 5.11 (s, 2 H, OCH_2Ar), 4.07 (s, 2 H, oxazoline CH_2), 2.34 (s, 3 H, $ArCCH_3$), 1.38 (s, 6 H, oxazoline CH_3). ^{13}C NMR (125 MHz): δ = 161.2 (C), 157.3 (C), 135.5 (C), 134.8 (C), 131.9 (CH), 131.1 (CH), 129.9 (CH), 127.7 (CH), 127.6 (CH), 125.7 (CH), 120.6 (CH), 118.4 (C), 113.3 (CH), 78.8 (oxazoline CH_2), 68.9 (OCH_2Ar), 67.4 (C), 28.3 (oxazoline CH_3), 18.8 ($ArCH_3$). HRMS (NSI^+): *m/z* calcd for $C_{19}H_{21}NO_2Na$ $[M+Na]^+$: 318.1465; found: 318.1459.

4,4-Dimethyl-2-(2-((4-nitrobenzyl)oxy)phenyl)-4,5-dihydrooxazole 5h

The same procedure as for **5a** using 2-(4,4-dimethyl-4,5-dihydrooxazol-2-yl)phenol **4** (0.57 g, 2.98 mmol), sodium hydride (0.12 g, 3.00 mmol) and 4-nitrobenzyl bromide (0.65 g, 3.01 mmol) in DMF (10 mL) gave, after recrystallisation (EtOAc/hexane), **5h** (0.66 g, 68%) as yellow crystals, mp 126–128 °C. IR: 2970, 2901, 1632, 1508, 1441, 1339, 1267, 1040, 968, 841, 735, 679 cm^{-1}. ^1H NMR (400 MHz): δ = 8.25 (d, *J* = 8.8 Hz, 2 H), 7.80 (d, *J* = 8.8 Hz, 2 H), 7.78 (dd, *J* = 7.6, 1.6 Hz, 1 H), 7.45–7.40 (m, 1 H), 7.06–7.02 (m, 1 H), 7.00 (d, *J* = 8.4 Hz, 1 H), 5.26 (s, 2 H, OCH_2Ar), 4.11 (s, 2 H, oxazoline CH_2), 1.44 (s, 6 H, CH_3). ^{13}C NMR (125 MHz): δ = 160.4 (C), 156.7 (C), 147.3 (CNO_2), 144.6 (C), 132.1 (CH), 131.4 (CH), 127.2 (2 CH), 123.6 (2 CH), 121.2 (CH), 118.3 (C), 113.1 (CH), 78.6 (oxazoline CH_2), 69.2 (OCH_2Ar), 67.9 (C), 28.6 (CH_3). HRMS (NSI^+): *m/z* calcd for $C_{18}H_{19}N_2O_4$ $[M+H]^+$: 327.1339; found: 327.1338.

4,4-Dimethyl-2-(2-((3-nitrobenzyl)oxy)phenyl)-4,5-dihydrooxazole 5i

The same procedure as for **5a** using 2-(4,4-dimethyl-4,5-dihydrooxazol-2-yl)phenol **4** (0.57 g, 2.98 mmol), sodium hydride (0.12 g, 3.00 mmol) and 3-nitrobenzyl bromide (0.65 g, 3.01 mmol) in DMF (10 mL) gave, after recrystallisation (EtOAc/hexane), **5i** (0.55 g, 57%) as pale yellow crystals, mp 90–92 °C. IR: 2970, 2901, 1636, 1526, 1497, 1447, 1346, 1258, 1030, 810, 727, 685 cm^{-1}. ^{1}H NMR (400 MHz): δ = 8.63–8.62 (m, 1 H), 8.18–8.16 (m, 1 H), 7.86–7.83 (m, 1 H), 7.81 (dd, *J* = 7.8, 1.8 Hz, 1 H), 7.55 (t, *J* = 8.0 Hz, 1 H), 7.46–7.41 (m, 1 H), 7.07–7.01 (m, 2 H), 5.24 (s, 2 H, OCH_2Ar), 4.17 (s, 2 H, oxazoline CH_2), 1.44 (s, 6 H, CH_3). ^{13}C NMR (125 MHz): δ = 160.7 (C), 156.7 (C), 148.5 (CNO_2), 139.3 (C), 132.3 (CH), 132.1 (CH), 131.5 (CH), 129.1 (CH), 122.5 (CH), 121.7 (CH), 121.2 (CH), 118.4 (C), 113.0 (CH), 78.8 (oxazoline CH_2), 68.9 (OCH_2Ar), 67.7 (C), 28.4 (CH_3). HRMS (NSI^+): *m/z* calcd for $C_{18}H_{19}N_2O_4$ $[M+H]^+$: 327.1339; found: 327.1339.

4,4-Dimethyl-2-(2-((2-nitrobenzyl)oxy)phenyl)-4,5-dihydrooxazole 5j

The same procedure as for **5a** using 2-(4,4-dimethyl-4,5-dihydrooxazol-2-yl)phenol **4** (0.57 g, 2.98 mmol), sodium hydride (0.12 g, 3.00 mmol) and 2-nitrobenzyl bromide (0.65 g, 3.01 mmol) in DMF (10 mL) gave, after recrystallisation (EtOAc/hexane), **5j** (0.56 g, 58%) as light sensitive tan-coloured crystals, mp 124–127 °C. IR: 2963, 2887, 1639, 1520, 1497, 1339, 1261, 1038, 970, 862, 733, 681, 665 cm^{-1}. ^{1}H NMR (400 MHz): δ = 8.58 (dd, *J* = 7.8, 1.0 Hz, 1 H), 8.21 (dd, *J* = 8.4, 1.2 Hz, 1 H), 7.80 (dd, *J* = 7.8, 1.8 Hz, 1 H), 7.74–7.70 (m, 1 H), 7.52–7.44 (m, 2 H), 7.13 (dd, *J* = 8.4, 0.8 Hz, 1 H), 7.04 (td, *J* = 7.6, 1.0 Hz, 1 H), 5.57 (s, 2 H, OCH_2Ar), 4.12 (s, 2 H, oxazoline CH_2), 1.46 (s, 6 H, CH_3). ^{13}C NMR (125 MHz): δ = 160.4 (C), 156.7 (C), 146.2 (CNO_2), 134.14 (C), 134.10 (CH), 132.3 (CH), 131.2 (CH), 129.4 (CH), 128.0 (CH), 124.7 (CH), 121.0 (CH), 117.8 (C), 113.0 (CH), 78.4 (oxazoline CH_2), 68.0 (C), 67.6 (OCH_2Ar), 28.6 (CH_3). HRMS (NSI^+): *m/z* calcd for $C_{18}H_{19}N_2O_4$ $[M+H]^+$: 327.1339; found: 327.1341.

2-((2-(4-Fluorophenyl)benzofuran-3-yl)amino)-2-methylpropan-1-ol 6a

The same procedure as for **3** using *n*-butyllithium (0.66 mL, 1.65 mmol), 2-(2-((4-fluorobenzyl)oxy)phenyl)-4,4-dimethyl-4,5-dihydrooxazole **5a** (0.1506 g, 0.50 mmol) and potassium *tert*-butoxide (0.1874 g, 1.67 mmol) in dry THF (5 mL) gave, after purification by repeated preparative TLC (SiO_2, Et_2O/hexane 7:3 then EtOAc/hexane 2:3), **6a** (18.3 mg, 12%) as a pale yellow oil. IR: 1605, 1508, 1450, 1258, 1231, 1153, 1061, 837, 752 cm^{-1}. ^{1}H NMR (500 MHz): δ = 8.12 (dd, *J* = 8.8, 5.3 Hz, 2 H), 7.64–7.62 (m, 1 H), 7.45 (d, *J* = 7.5 Hz, 1 H), 7.28–7.26 (m, 1 H), 7.25–7.22 (m, 1 H), 7.14 (t, *J* = 8.8 Hz, 2 H), 3.44 (s, 2 H, CH_2), 1.07 (s, 6 H, CH_3). ^{13}C NMR (125 MHz): δ = 162.3 (d, J_{CF} = 247 Hz, CF), 152.9 (C–O), 148.0 (C–O), 129.6 (C), 128.4 (d, J_{CF} = 7.9 Hz, 2 CH), 127.5 (d, J_{CF} = 3.3 Hz, C), 124.4 (CH), 122.6 (CH), 121.9 (C), 119.5 (CH), 115.5 (d, J_{CF} = 21.5 Hz, 2 CH), 111.2 (CH), 70.5 (CH_2), 58.2 (C), 24.6 (CH_3). ^{19}F NMR (376 MHz): δ = –112.6. HRMS (NSI^+): *m/z* calcd for $C_{18}H_{19}FNO_2$ $[M+H]^+$: 300.1394; found: 300.1392.

2-((2-(4-Methoxyphenyl)benzofuran-3-yl)amino)-2-methylpropan-1-ol 6b

The same procedure as for **3** using *n*-butyllithium (0.66 mL, 1.65 mmol), 2-(2-((4-methoxybenzyl)oxy)phenyl)-4,4-dimethyl-4,5-dihydrooxazole **5b** (0.1567 g, 0.50 mmol) and potassium *tert*-butoxide (0.1880 g, 1.68 mmol) in dry THF (5 mL) gave, after purification by preparative TLC (SiO_2, Et_2O/hexane 7:3), at R_f 0.75, **6b** (0.1033 g, 66%) as a yellow oil. IR: 3329, 2967, 1605, 1510, 1452, 1248, 1165, 1026, 827, 748 cm^{-1}. ^1H NMR (400 MHz): δ = 8.01 (d, *J* = 8.8 Hz, 2 H), 7.61–7.58 (m, 1 H), 7.43–7.41 (m, 1 H), 7.26–7.18 (m, 2 H), 6.96 (d, *J* = 8.8 Hz, 2 H), 3.82 (s, 3 H, OCH_3), 3.40 (s, 2 H, CH_2), 2.86 (br s, 2 H, NH and OH), 1.05 (s, 6 H, CH_3). ^{13}C NMR (125 MHz): δ = 159.3 (C–O), 152.7 (C–O), 148.9 (C–O), 129.8 (C), 128.0 (2 CH), 123.9 (CH), 123.8 (C), 122.4 (CH), 120.8 (C), 119.3 (CH), 113.9 (2 CH), 111.0 (CH), 70.3 (CH_2), 58.0 (C), 55.2 (OCH_3), 24.6 (CH_3). HRMS (NSI^+): *m/*z calcd for $C_{19}H_{22}NO_3$ $[M+H]^+$: 312.1594; found: 312.1596.

2-((2-(3-Methoxyphenyl)benzofuran-3-yl)amino)-2-methylpropan-1-ol 6c

The same procedure as for **3** using *n*-butyllithium (0.66 mL, 1.65 mmol), 2-(2-((3-methoxybenzyl)oxy)phenyl)-4,4-dimethyl-4,5-dihydrooxazole **5c** (0.1553 g, 0.50 mmol) and potassium *tert*-butoxide (0.1870 g, 1.67 mmol) in dry THF (5 mL) gave, after purification by repeated preparative TLC (SiO_2, Et_2O then Et_2O/hexane 7:3), **6c** (20.2 mg, 13%) as a yellow oil. IR: 2970, 1603, 1487, 1452, 1273, 1206, 1038, 748 cm^{-1}. ^1H NMR (500 MHz): δ = 7.68–7.63 (m, 3 H), 7.46 (d, *J* = 8.0 Hz, 1 H), 7.36 (t, *J* = 8.0 Hz, 1 H), 7.30–7.27 (m, 1 H), 7.23 (td, *J* = 7.5, 1.0 Hz, 1 H), 6.89 (ddd, *J* = 8.0, 2.5, 1.0 Hz, 1 H), 3.88 (s, 3 H, OCH_3), 3.44 (s, 2 H, CH_2), 2.46 (br s, 2 H, NH and OH), 1.10 (s, 6 H, CH_3). ^{13}C NMR (125 MHz): δ = 159.6 (C–O), 152.9 (C–O), 148.4 (C–O), 132.4 (C), 129.6 (CH), 129.5 (C), 124.5 (CH), 122.55 (CH), 122.46 (C), 119.6 (CH), 118.9 (CH), 114.2 (CH), 111.7 (CH), 111.3 (CH), 70.4 (CH_2), 58.2 (C), 55.3 (OCH_3), 24.8 (CH_3). HRMS (NSI^+): *m/*z calcd for $C_{19}H_{22}NO_3$ $[M+H]^+$: 312.1594; found: 312.1597.

2-((2-(2-Methoxyphenyl)benzofuran-3-yl)amino)-2-methylpropan-1-ol 6d

The same procedure as for **3** using *n*-butyllithium (0.66 mL, 1.65 mmol), 2-(2-((2-methoxybenzyl)oxy)phenyl)-4,4-dimethyl-4,5-dihydrooxazole **5d** (0.1551 g, 0.50 mmol) and potassium *tert*-butoxide (0.1872 g, 1.67 mmol) in dry THF (5 mL) gave, after purification by preparative TLC (SiO_2, Et_2O/hexane 4:1), at R_f 0.85, **6d** (16.3 mg, 11%) as a pale yellow oil. IR: 3275, 2968, 2936, 1601, 1491, 1462, 1244, 1198, 1020, 750 cm^{-1}. ^1H NMR (400 MHz): δ = 7.72–7.68 (m, 2 H), 7.46–7.39 (m, 2 H), 7.30–7.22 (m, 2 H), 7.13 (td, *J* = 7.6, 1.2 Hz, 1 H), 7.05 (d, *J* = 8.4 Hz, 1 H), 3.94 (s, 3 H, OCH_3), 3.35 (s, 2 H, CH_2), 3.22 (br s, 2 H, NH and OH), 0.94 (s, 6 H, CH_3). ^{13}C NMR (125 MHz): δ = 155.6 (C–O), 154.2 (C–O), 145.8 (C–O), 130.4 (CH), 130.1 (CH), 129.1 (C), 124.2 (CH), 123.9 (C), 122.4 (CH), 121.5 (CH), 120.3 (C), 120.1 (CH), 111.8 (CH), 111.1 (CH), 69.8 (CH_2), 57.6 (C), 56.0 (OCH_3), 24.7 (CH_3). HRMS (NSI^+): *m/*z calcd for $C_{19}H_{22}NO_3$ $[M+H]^+$: 312.1594; found: 312.1591.

2-((2-(2-Methoxynaphthalen-1-yl)benzofuran-3-yl)amino)-2-methylpropan-1-ol 6e

The same procedure as for **3** using *n*-butyllithium (0.66 mL, 1.65 mmol), 2-(2-((2-methoxynaphthalen-1-yl)methoxy)phenyl)-4,4-dimethyl-4,5-dihydrooxazole **5e** (0.1815 g, 0.50 mmol) and potassium *tert*-butoxide (0.1854 g, 1.65 mmol) in dry THF (5 mL) gave, after purification by preparative TLC (SiO_2, Et_2O/hexane 7:3), at R_f 0.20, **6e** (85.3 mg, 47%) as a tan-coloured solid, mp 129–132 °C. IR: 3308, 3188, 2970, 1591, 1506, 1452, 1341, 1254, 1182, 1150, 1119, 1067, 810, 752 cm^{-1}. ^1H NMR (400 MHz): δ = 7.96 (d, *J* = 8.8 Hz, 1 H), 7.83 (d, *J* = 8.0 Hz, 1 H),

7.77–7.72 (m, 2 H), 7.50–7.43 (m, 2 H), 7.40–7.37 (m, 1 H), 7.35 (d, *J* = 9.2 Hz, 1 H), 7.31–7.28 (m, 2 H), 3.91 (s, 3 H, OCH_3), 3.27 and 3.17 (AB pattern, *J* = 10.4 Hz, 2 H, CH_2), 2.42 (br s, 1 H, NH), 0.92 (s, 3 H, CH_3), 0.86 (s, 3 H, CH_3). ^{13}C NMR (125 MHz): δ = 155.3 (C–O), 154.4 (C–O), 144.6 (C–O), 133.4 (C), 131.9 (CH), 129.0 (C), 128.7 (C), 128.1 (CH), 127.5 (CH), 125.5 (C), 124.9 (CH), 124.2 (CH), 124.0 (CH), 122.4 (CH), 119.9 (CH), 113.1 (CH), 112.8 (C), 111.3 (CH), 69.5 (CH_2), 56.9 (C), 56.8 (OCH_3), 25.0 (CH_3), 24.3 (CH_3). HRMS (NSI$^+$): *m/*z calcd for $C_{23}H_{24}NO_3$ $[M+H]^+$: 362.1751; found: 362.1746.

2-((1-Hydroxy-2-methylpropan-2-yl)carbamoyl)phenyl 4-methylbenzoate 7a

The same procedure as for **3** using *n*-butyllithium (0.66 mL, 1.65 mmol), 4,4-dimethyl-2-(2-((4-methylbenzyl)oxy)phenyl)-4,5-dihydrooxazole **5f** (0.1483 g, 0.50 mmol) and potassium *tert*-butoxide (0.1873 g, 1.67 mmol) in dry THF (5 mL) gave, after purification by preparative TLC (SiO_2, Et_2O/hexane 4:1), at R_f 0.40, **7a** (28.0 mg, 17%) as a pale yellow oil. IR: 3348, 2928, 1753, 1639, 1609, 1523, 1449, 1261, 1177, 1096, 1059, 745 cm^{-1}. ^{1}H NMR (400 MHz): δ = 8.09 (d, *J* = 8.4 Hz, 2 H), 7.77 (dd, *J* = 7.6, 1.6 Hz, 1 H), 7.51 (ddd, *J* = 8.0, 7.6, 1.6 Hz, 1 H), 7.37–7.32 (m, 3 H), 7.19 (dd, *J* = 8.2, 1.0 Hz, 1 H), 6.37 (br s, 1 H, NH), 4.44 (br s, 1 H, OH), 3.53 (s, 2 H, CH_2), 2.47 (s, 3 H, $ArCH_3$), 1.16 (s, 6 H, CH_3). ^{13}C NMR (125 MHz): δ = 166.5 (C=O), 165.4 (C=O), 147.7 (C), 145.3 (C), 131.9 (CH), 130.3 (2 CH), 129.7 (CH), 129.6 (2 CH), 129.4 (C), 126.5 (CH), 125.8 (C), 123.0 (CH), 69.8 (CH_2), 56.5 (C), 24.4 (CH_3), 21.8 ($ArCH_3$). HRMS (NSI$^+$): *m/*z calcd for $C_{19}H_{22}NO_4$ $[M+H]^+$: 328.1543; found: 328.1545.

2-((1-Hydroxy-2-methylpropan-2-yl)carbamoyl)phenyl 2-methylbenzoate 7b

The same procedure as for **3** using *n*-butyllithium (0.66 mL, 1.65 mmol), 4,4-dimethyl-2-(2-((2-methylbenzyl)oxy)phenyl)-4,5-dihydrooxazole **5g** (0.1482 g, 0.50 mmol) and potassium *tert*-butoxide (0.1850 g, 1.65 mmol) in dry THF (5 mL) gave, after purification by repeated preparative TLC (SiO_2, Et_2O/hexane 4:1 then Et_2O/hexane 1:1), **7b** (8.3 mg, 5%) as a pale yellow oil. IR: 3352, 2970, 2930, 1740, 1639, 1524, 1456, 1240, 1200, 1043, 1026, 737 cm^{-1}. ^{1}H NMR (400 MHz): δ = 8.21 (d, *J* = 7.6 Hz, 1 H), 7.80 (dd, *J* = 7.8, 1.8 Hz, 1 H), 7.55–7.50 (m, 2 H), 7.38–7.33 (m, 3 H), 7.20 (dd, *J* = 8.2, 1.0 Hz, 1 H), 6.38 (br s, 1 H, NH), 4.36 (br s, 1 H, OH), 3.54 (s, 2 H, CH_2), 2.67 (s, 3 H, $ArCH_3$), 1.16 (s, 6 H, CH_3). ^{13}C NMR (125 MHz): δ = 166.5 (C=O), 165.5 (C=O), 147.7 (C), 141.9 (C), 133.5 (CH), 132.2 (CH), 131.9 (CH), 131.3 (CH), 129.7 (CH), 129.2 (C), 127.3 (C), 126.4 (CH), 126.2 (CH), 123.2 (CH), 69.9 (CH_2), 56.6 (C), 24.4 (CH_3), 22.0 ($ArCH_3$). HRMS (NSI$^+$): *m/*z calcd for $C_{19}H_{22}NO_4$ $[M+H]^+$: 328.1543; found: 328.1537.

4,4-Dimethyl-2-(2-(1-phenylethoxy)phenyl)-4,5-dihydrooxazole 8

The same procedure as for **5a** using 2-(4,4-dimethyl-4,5-dihydrooxazol-2-yl)phenol **4** (0.57 g, 2.98 mmol), sodium hydride (0.12 g, 3.00 mmol) and (1-bromoethyl)benzene (0.41 mL, 0.56 g, 3.00 mmol) in DMF (10 mL) gave, after purification by column chromatography (SiO_2, Et_2O/hexane 1:1), at R_f 0.50, **8** (0.56 g, 64%) as a colourless oil. IR: 2968, 2929, 1647, 1600, 1491, 1451, 1350, 1314, 1245, 1125, 1068, 1037, 758, 702 cm^{-1}. ^{1}H NMR (500 MHz): δ = 7.62 (dd, *J* = 7.5, 2.0 Hz, 1 H), 7.42–7.40 (m, 2 H), 7.34–7.30 (m, 2 H), 7.26–7.20 (m, 2 H), 6.91–6.88 (m, 1 H), 6.78 (d, *J* = 8.5 Hz, 1 H), 5.33 (q, *J* = 6.5 Hz, 1 H, C***H***CH_3), 4.13 (s, 2 H, CH_2), 1.63 (d, *J* = 6.5 Hz, 3 H, CHC***H***$_3$), 1.42 (s, 3 H, CH_3),

1.41 (s, 3 H, CH_3). ^{13}C NMR (125 MHz): δ = 161.9 (C), 156.5 (C), 143.1 (C), 131.5 (CH), 131.0 (CH), 128.5 (2 CH), 127.4 (CH), 125.7 (2 CH), 120.6 (CH), 119.5 (C), 115.4 (CH), 79.1 (CH_2), 77.3 (***C***HCH_3), 67.3 (C), 28.42 (CH_3), 28.37 (CH_3), 24.2 (CH***C***H_3). HRMS (NSI$^+$): *m/*z calcd for $C_{19}H_{21}NO_2Na$ $[M+Na]^+$: 318.1465; found: 318.1464.

2,4',4'-Trimethyl-2-phenyl-2*H*-spiro[benzofuran-3,2'-oxazolidine] 9

The same procedure as for **3** using *n*-butyllithium (0.66 mL, 1.65 mmol), 4,4-dimethyl-2-(2-(1-phenylethoxy)phenyl)-4,5-dihydrooxazole **8** (0.1482 g, 0.50 mmol) and potassium *tert*-butoxide (0.1862 g,) in dry THF (5 mL) gave, after purification by repeated preparative TLC (Al_2O_3, Et_2O/hexane 3:2), at R_f 0.75, **9** (39.0 mg, 26%) as a colourless oil. ν_{max}/cm^{-1} 3360, 2968, 1601, 1464, 1379, 1242, 895, 750, 698. ^{1}H NMR revealed a 5:3 mixture of diastereomers. ^{1}H NMR (400 MHz, major diastereomer): δ = 7.61–6.92 (m, 9 H), 3.84 and 3.60 (AB pattern, *J* = 8.0 Hz, 2 H, CH_2), 1.94 (br s, 1 H, NH), 1.85 (s, 3 H, OC(Ph)CH_3), 1.32 (s, 3 H, CH_3), 0.96 (s, 3 H, CH_3). ^{13}C NMR (125 MHz, major diastereomer): δ = 158.4 (C–O), 141.4 (C), 130.7 (C), 130.5 (CH), 128.2 (2 CH), 127.7 (CH), 126.6 (2 CH), 124.3 (CH), 121.3 (CH), 110.7 (CH), 105.0 (spiro C), 93.26 (O***C***(Me)Ph), 78.1 (CH_2), 58.5 (C), 28.3 (CH_3), 26.7 (CH_3), 21.4 (OC(Ph)***C***H_3). ^{1}H NMR (400 MHz, minor diastereomer): δ = 7.61–6.92 (m, 9 H), 3.34 and 2.69 (AB pattern, *J* = 8.0 Hz, 2 H, CH_2), 1.94 (br s, 1 H, NH), 1.70 (s, 3 H, OC(Ph)CH_3), 1.41 (s, 3 H, CH_3), 1.13 (s, 3 H, CH_3). ^{13}C NMR (125 MHz, minor diastereomer): δ = 158.8 (C–O), 139.6 (C), 130.9 (CH), 130.1 (C), 127.4 (CH), 127.3 (2 CH), 126.8 (2 CH), 123.7 (CH), 120.9 (CH), 111.4 (CH), 104.3 (spiro C), 93.30 (O***C***(Me)Ph), 76.7 (CH_2), 57.9 (C), 28.5 (CH_3), 27.6 (CH_3), 22.8 (OC(Ph)***C***H_3). HRMS (NSI$^+$): *m/*z calcd for $C_{19}H_{22}NO_2$ $[M+H]^+$: 296.1645; found: 296.1640.

2-(2-(Benzhydryloxy)phenyl)-4,4-dimethyl-4,5-dihydrooxazole 10

The same procedure as for **5a** using 2-(4,4-dimethyl-4,5-dihydrooxazol-2-yl)phenol **4** (0.57 g, 2.98 mmol), sodium hydride (0.13 g, 3.25 mmol) and benzhydryl bromide (0.75 g, 3.03 mmol) in DMF (10 mL) gave, after purification by column chromatography (SiO_2, Et_2O/hexane 1:1), at R_f 0.55, **10** (0.53 g, 50%) as a colourless oil. IR: 2965, 1647, 1599, 1491, 1449, 1242, 1036, 745, 694 cm^{-1}. ^{1}H NMR (500 MHz): δ = 7.66 (dd, *J* = 7.5, 1.5 Hz, 1 H), 7.54 (d, *J* = 7.5 Hz, 4 H), 7.32–7.29 (m, 4 H), 7.23–7.19 (m, 3 H), 6.90 (t, *J* = 7.5 Hz, 1 H), 6.84 (d, *J* = 8.0 Hz, 1 H), 6.26 (s, 1 H, $CHPh_2$), 4.11 (s, 2 H, CH_2), 1.41 (s, 6 H, CH_3). ^{13}C NMR (100 MHz): δ = 161.6 (C=N), 156.2 (C–O), 141.6 (2 C), 131.5 (CH), 131.0 (CH), 128.5 (4 CH), 127.5 (2 CH), 126.5 (4 CH), 120.6 (CH), 119.2 (C), 114.9 (CH), 82.1 ($CHPh_2$), 79.0 (CH_2), 67.4 (C), 28.5 (CH_3). HRMS (NSI$^+$): *m/*z calcd for $C_{24}H_{23}NO_2Na$ $[M+Na]^+$: 380.1621; found: 380.1616.

2-((2,2-Diphenylbenzofuran-3(2*H*)-ylidene)amino)-2-methylpropan-1-ol 11

The same procedure as for **3** using *n*-butyllithium (0.66 mL, 1.65 mmol), 2-(2-(benzhydryloxy)phenyl)-4,4-dimethyl-4,5-dihydrooxazole **10** (0.1807 g, 0.51 mmol) and potassium *tert*-butoxide (0.1865 g, 1.66 mmol) in dry THF (5 mL) gave, after purification by preparative TLC (Al_2O_3, Et_2O/hexane 3:2), at R_f 0.75, **11** (0.1307 g, 72%) as pale yellow crystals, mp 100–104 °C. IR: 3482, 2968, 1661, 1601, 1585, 1460, 1250, 1045, 989, 914, 750, 696, 610 cm^{-1}. ^{1}H NMR (400 MHz): δ = 7.80 (dd, *J* = 8.0, 0.8 Hz, 1 H), 7.44–7.39 (m, 5 H), 7.32–7.25 (m, 6 H), 7.14 (d, *J* = 8.0 Hz, 1 H), 7.02–6.98 (m, 1 H), 3.41 (d, *J* = 5.6 Hz, 2 H, CH_2), 2.80 (t, *J* = 5.6 Hz, 1 H, OH), 1.39 (s, 6 H, CH_3). ^{13}C NMR (125

MHz): δ = 167.4 (C), 167.2 (C), 141.8 (2 C), 134.0 (CH), 128.7 (CH), 127.9 (4 CH), 127.8 (2 CH), 127.3 (4 CH), 121.0 (CH), 117.6 (C), 113.0 (CH), 93.5 ($OCPh_2$), 73.9 (CH_2), 58.2 (C), 21.0 (CH_3). HRMS (NSI^+): *m/*z calcd for $C_{24}H_{24}NO_2$ $[M+H]^+$: 358.1802; found: 358.1804.

2-(Allyloxy)-*N*-(1-hydroxy-2-methylpropan-2-yl)benzamide E

The same procedure as for **B** using 2-(allyloxy)benzoyl chloride[8] (34.62 g, 0.176 mol) in CH_2Cl_2 (150 mL) and 2-amino-2-methylpropan-1-ol (31.39 g, 0.352 mol) in CH_2Cl_2 (150 mL) gave **E** (42.78 g, 97%) as a colourless oil which was used without further purification. IR: 3371, 2931, 1746, 1635, 1539, 1482, 1312, 1230, 1102, 1064, 996, 938, 879, 756 cm^{-1}. ^1H NMR (500 MHz): δ = 8.24 (br s, 1 H, NH), 8.17 (dd, *J* = 8.0, 2.0 Hz, 1 H), 7.44 (ddd, *J* = 8.5, 7.5, 2.0 Hz, 1 H), 7.10–7.07 (m, 1 H), 6.96 (d, *J* = 8.5 Hz, 1 H), 6.12 (ddt, *J* = 17.0, 10.5, 6.0 Hz, 1 H, C***H***=CH_2), 5.50 (dq, *J* = 17.0, 1.3 Hz, 1 H, CH=C***H***H), 5.42 (dq, *J* = 10.5, 1.3 Hz, 1 H, CH=CH***H***), 5.37 (t, *J* 6.0, 1 H, OH), 4.65 (dt, *J* = 6.0, 1.3 Hz, 2 H, OC***H***$_2$CH=CH_2), 3.67 (d, *J* = 6.0 Hz, 2 H, C***H***$_2$OH), 1.38 (s, 6 H, CH_3). ^{13}C NMR (125 MHz): δ = 165.7 (C=O), 156.4 (C–O), 132.9 (CH), 132.1 (CH), 131.7 (CH), 121.7 (C), 121.6 (CH), 120.2 (CH=***C***H_2), 112.6 (CH), 71.1 (OCH_2), 70.1 (OCH_2), 56.3 (C), 24.9 (CH_3). HRMS (ESI^+): *m/*z calcd for $C_{14}H_{19}NNaO_3$ $[M+Na]^+$: 272.1257; found: 272.1250.

2-(2-(Allyloxy)phenyl)-4,4-dimethyl-4,5-dihydrooxazole 12

The same procedure as for **1** using thionyl chloride (13.5 mL, 22.02 g, 0.185 mol) and 2-(allyloxy)-*N*-(1-hydroxy-2-methylpropan-2-yl)benzamide **E** (42.78 g, 0.172 mol) in CH_2Cl_2 (150 mL) gave, after purification by kugelrohr distillation (240 °C/6.7 Torr), **12** (35.09 g, 88%) as an orange oil. IR: 3080, 2968, 1648, 1601, 1496, 1451, 1351, 1317, 1123, 1039, 926, 753, 691 cm^{-1}. ^1H NMR (400 MHz): δ = 7.71 (dd, *J* = 7.8, 1.8 Hz, 1 H), 7.39–7.34 (m, 1 H), 6.96 (td, *J* = 7.6, 0.8 Hz, 1 H), 6.92 (d, *J* = 8.4 Hz, 1 H), 6.04 (ddt, *J* = 17.2, 10.6, 4.6 Hz, 1 H, C***H***=CH_2), 5.56 (dq, *J* = 17.2, 1.6 Hz, 1 H, CH=C***H***H), 5.27 (dq, *J* = 10.6, 1.6 Hz, 1 H, CH=CH***H***), 4.59 (dt, *J* = 4.6, 1.6 Hz, 2 H, OC***H***$_2$CH=CH_2), 4.09 (s, 2 H, CH_2), 1.39 (s, 6 H, CH_3). ^{13}C NMR (100 MHz): δ = 161.2 (C=N), 157.2 (C–O), 132.8 (CH), 131.8 (CH), 131.1 (CH), 120.5 (CH), 118.4 (C), 116.7 (CH=***C***H_2), 113.3 (CH), 78.9 (oxazoline CH_2), 69.2 (allyl OCH_2), 67.4 (C), 28.3 (CH_3). The ^1H NMR spectral data was in accordance with that previously reported.[9]

2-Methyl-2-((2-vinylbenzofuran-3-yl)amino)propan-1-ol 13

The same procedure as for **3** using *n*-butyllithium (19.8 mL, 49.5 mmol), 2-(2-(allyloxy)phenyl)-4,4-dimethyl-4,5-dihydrooxazole **12** (3.49 g, 15.1 mmol) and potassium *tert*-butoxide (5.58 g, 49.7 mmol) gave, after purification by column chromatography (Al_2O_3, gradient elution, Et_2O/hexane 3:2 to Et_2O), **13** (2.19 g, 63%) as a viscous orange oil. IR: 3341, 2967, 2932, 1605, 1454, 1379, 1254, 1186, 1045, 908, 729 cm^{-1}. ^1H NMR (500 MHz): δ = 7.56–7.54 (m, 1 H), 7.37 (d, *J* = 8.0 Hz, 1 H), 7.26–7.22 (m, 1 H), 7.18–7.15 (m, 1 H), 6.77 (dd, *J* = 17.5, 11.0 Hz, 1 H, C***H***=CH_2), 5.88 (dd, *J* = 17.5, 1.5 Hz, 1 H, CH=C***H***H), 5.31 (dd, *J* = 11.0, 1.5 Hz, 1 H, CH=CH***H***), 3.45 (s, 2 H, C***H***$_2$OH), 3.17 (br s, 2 H, NH and OH), 1.12 (s, 6 H, CH_3). ^{13}C NMR (125 MHz): δ = 153.3 (C), 148.5 (C), 128.6 (C), 124.8 (CH), 123.0 (C), 122.6 (CH), 122.4 (CH), 119.6 (CH), 113.9 (CH=***C***H_2), 111.0 (CH), 69.7 (CH_2OH), 57.5 (C), 24.7 (CH_3). HRMS (ESI^+): *m/*z calcd for $C_{14}H_{18}NO_2$ $[M+H]^+$: 232.1332; found: 232.1329.

2-Methyl-2-((2-(2,3,4,5-tetrachlorocyclohexa-2,4-dien-1-yl)benzofuran-3-yl)amino)propan-1-ol 14

A mixture of 2-methyl-2-((2-vinylbenzofuran-3-yl)amino)propan-1-ol **13** (0.40 g, 1.73 mmol) and tetrachlorothiophene *S*,*S*-dioxide[10] (0.44 g, 1.73 mmol) in toluene (20 mL) was heated under reflux for 6 h. After cooling to rt, the reaction mixture was evaporated and the crude residue was purified by column chromatography (SiO_2, Et_2O/hexane 3:2) to give, at R_f 0.60, **14** (0.1319 g, 18%) as brown crystals, mp 99–102 °C. IR: 3337, 2927, 1603, 1566, 1454, 1206, 1079, 814, 748, 703, 664, 608 cm^{-1}. ^1H NMR (400 MHz): δ = 7.60 (ddd, *J* = 7.6, 1.6, 0.8 Hz, 1 H), 7.42–7.39 (m, 1 H), 7.30–7.26 (m, 1 H), 7.23 (td, *J* = 7.4, 1.2 Hz, 1 H), 4.53 (dd, *J* = 9.6, 9.2 Hz, 1 H, C***H***CH_2), 3.49 and 3.42 (AB pattern, *J* = 10.6 Hz, 2 H, CH_2OH), 3.19 (half AB pattern of d, J_{AB} = 17.2, J_{AX} = 9.6 Hz, 1 H, CHC***H***$_2$), 3.12 (half AB pattern of d, J_{AB} = 17.2, J_{BX} = 9.2 Hz, 1 H, CHC***H***$_2$), 2.44 (br s, 2 H, NH and OH), 1.18 (s, 3 H, CH_3), 1.16 (s, 3 H, CH_3). ^{13}C NMR (125 MHz): δ = 153.5 (C–O), 148.2 (C–O), 129.1 (C), 127.91 (C), 127.90 (C), 126.2 (C), 124.6 (CH), 123.7 (C), 123.2 (C), 122.7 (CH), 119.9 (CH), 111.6 (CH), 69.6 (CH_2OH), 56.9 (C), 38.6 (***C***HCH_2), 37.1 (CH***C***H_2), 25.2 (CH_3), 25.0 (CH_3). HRMS (NSI^+): *m/*z calcd for $C_{18}H_{18}{}^{35}Cl_3{}^{37}ClNO_2$ $[M+H]^+$: 422.0057; found: 422.0055.

2-(4,4-Dimethyl-4,5-dihydrooxazol-2-yl)phenol 4

Under a nitrogen atmosphere, *n*-butyllithium (2.5 M in hexane, 17.5 mL, 43.8 mmol) was added dropwise to a stirred mixture of 2-(2-(allyloxy)phenyl)-4,4-dimethyl-4,5-dihydrooxazole **12** (5.04 g, 21.8 mmol) and potassium *tert*-butoxide (5.35 g, 47.7 mmol) in dry toluene (220 mL). After stirring at rt for 2 h, the reaction mixture was poured into sat. aq. NH_4Cl (150 mL), the two layers were separated and the aqueous layer was re-extracted with Et_2O (2 × 50 mL). The combined organic layers were dried and evaporated and the crude residue was purified by column chromatography (SiO_2, Et_2O/hexane 7:3) to give, at R_f 0.90, after subsequent kugelrohr distillation (185 °C, 20 Torr), **4** (3.70 g, 89%) as a pale yellow oil. ^1H NMR (400 MHz): δ = 12.18 (br s, 1 H, OH), 7.63 (ddd, *J* = 8.0, 1.6, 0.4 Hz, 1 H), 7.36 (ddd, *J* = 8.4, 7.2, 2.0 Hz, 1 H), 7.00 (ddd, *J* = 8.4, 1.2, 0.4 Hz, 1 H), 6.86 (ddd, *J* = 7.6, 7.2, 1.2 Hz, 1 H), 4.10 (s, 2 H, CH_2), 1.40 (s, 6 H, CH_3). ^{13}C NMR (100 MHz): δ = 163.4 (C), 159.7 (C), 133.0 (CH), 127.8 (CH), 118.4 (CH), 116.5 (CH), 110.8 (C), 78.2 (CH_2), 67.0 (C), 28.4 (CH_3). The ^1H and ^{13}C NMR spectral data was in accordance with that previously reported.[9]

2-(Benzylthio)benzoyl chloride F

The same procedure as for **A** using thionyl chloride (2.4 mL, 3.91 g, 32.9 mmol) and 2-(benzylthio)benzoic acid[11] (4.03 g, 16.5 mmol) in toluene (30 mL) gave **F** (4.33 g, 100%) as pale yellow crystals which were used without further purification, mp 117–120 °C (lit.[12] 121–122 °C). ^1H NMR (500 MHz): δ = 8.29 (dd, *J* = 8.0, 1.0 Hz, 1 H), 7.52–7.49 (m, 1 H), 7.42–7.37 (m, 3 H), 7.33 (t, *J* = 7.5 Hz, 2 H), 7.29–7.23 (m, 2 H), 4.19 (s, 2 H, CH_2). ^{13}C NMR (125 MHz): δ = 166.3 (C=O), 144.3 (C–S), 135.3 (CH), 135.2 (C), 134.3 (CH), 129.7 (C), 129.0 (2 CH), 128.7 (2 CH), 127.6 (CH), 125.8 (CH), 124.3 (CH), 37.2 (CH_2). HRMS (ESI^+): *m/*z calcd for $C_{14}H_{11}OS$ $[M–Cl]^+$: 227.0525; found: 227.0521.

2-(Benzylthio)-*N*-(1-hydroxy-2-methylpropan-2-yl)benzamide G

The same procedure as for **B** using 2-(benzylthio)benzoyl chloride **F** (4.33 g, 16.5 mmol) in CH_2Cl_2 (80 mL) and 2-amino-2-methylpropan-1-ol (2.97 g, 33.3 mmol) in CH_2Cl_2 (40 mL) gave **G** (4.82 g, 93%) as a pale yellow solid which was used without further purification, mp 115–118 °C. IR: 1713, 1628, 1175, 1066, 721, 653 cm^{-1}. ^1H NMR (500 MHz): δ = 7.56 (dd, *J* = 7.5, 2.0 Hz, 1 H), 7.36 (dd, *J* = 7.8, 1.3 Hz, 1 H), 7.30 (td, *J* = 7.5, 1.5 Hz, 1 H), 7.28–7.22 (m, 4 H), 7.19–7.17 (m, 2 H), 6.49 (br s, 1 H, NH), 4.28 (br s, 1 H, OH), 4.09 (s, 2 H, SCH_2), 3.68 (s, 2 H, C***H***$_2$OH), 1.34 (s, 6 H, CH_3). ^{13}C NMR (125 MHz): δ = 168.7 (C=O), 138.3 (C), 136.9 (C), 132.7 (C), 132.4 (CH), 130.4 (CH), 128.7 (2 CH), 128.6 (CH), 128.5 (2 CH), 127.3 (CH), 127.2 (CH), 70.1 (CH_2OH), 56.8 (C), 40.2 (SCH_2), 24.5 (CH_3). HRMS (ESI^+): *m/*z calcd for $C_{18}H_{21}NO_2SNa$ $[M+Na]^+$: 338.1185; found: 338.1178.

2-(2-(Benzylthio)phenyl)-4,4-dimethyl-4,5-dihydrooxazole 15

The same procedure as for **1** using thionyl chloride (1.4 mL, 2.28 g, 19.2 mmol) and 2-(benzylthio)-*N*-(1-hydroxy-2-methylpropan-2-yl)benzamide **G** (4.82 g, 15.3 mmol) in CH_2Cl_2 (150 mL) gave, after recrystallisation (EtOAc/hexane), **15** (4.05 g, 89%) as colourless needles, mp 128–131 °C (lit.[13] 126–128 °C). IR: 1718, 1645, 1561, 1313, 1256, 1141, 1034, 967, 866, 818, 771, 736, 684, 654 cm^{-1}. ^1H NMR (500 MHz): δ = 7.72 (d, *J* = 7.0 Hz, 1 H), 7.39 (d, *J* = 7.0 Hz, 2 H), 7.32–7.28 (m, 4 H), 7.26–7.23 (m, 1 H), 7.17–7.14 (m, 1 H), 4.14 (s, 2 H, CH_2), 4.08 (s, 2 H, CH_2), 1.40 (s, 6 H, CH_3). HRMS (ESI^+): *m/*z calcd for $C_{18}H_{20}NOS$ $[M+H]^+$: 298.1260; found: 298.1253. The ^1H NMR spectral data was in accordance with that previously reported.[13]

2-Methyl-2-((2-phenylbenzo[*b*]thiophen-3-yl)amino)propan-1-ol 16

The same procedure as for **2** using *n*-butyllithium (10.1 mL, 25.3 mmol), 2-(2-(benzylthio)phenyl)-4,4-dimethyl-4,5-dihydrooxazole **15** (3.01 g, 10.1 mmol) and potassium *tert*-butoxide (2.87 g, 25.6 mmol) in dry THF (100 mL) gave, after recrystallisation (EtOAc/hexane), **16** (2.34 g, 78%) as pale yellow crystals, mp 106–109 °C. IR: 1651, 1609, 1562, 1504, 1431, 1227, 1018, 806, 733, 698 cm^{-1}. ^1H NMR (500 MHz): δ = 7.83 (d, *J* = 8.0 Hz, 1 H), 7.78 (d, *J* = 8.0 Hz, 1 H), 7.65–7.62 (m, 2 H), 7.48–7.45 (m, 2 H), 7.41–7.36 (m, 2 H), 7.35–7.32 (m, 1 H), 3.21 (s, 2 H, CH_2), 0.90 (s, 6 H, CH_3). ^{13}C NMR (75 MHz): δ = 139.3 (C), 137.1 (C), 134.7 (C), 133.9 (C), 133.7 (C), 129.4 (2 CH), 128.8 (2 CH), 128.0 (CH), 124.4 (CH), 124.0 (CH), 122.3 (2 CH), 70.3 (CH_2), 58.6 (C), 24.8 (CH_3). HRMS (ESI^+): *m/*z calcd for $C_{18}H_{20}NOS$ $[M+H]^+$: 298.1260; found: 298.1255.

Crystal data for **16**: $C_{18}H_{19}NOS$, M = 297.41, colourless prism, crystal dimensions 0.20 × 0.20 × 0.20 mm, monoclinic, space group $P2_1/c$, *a* = 11.976(2), *b* = 12.4118(15), *c* = 20.997(3) Å, β = 95.825(6)°, *V* = 3105.0(8) $Å^3$, *Z* = 8, D_c = 1.272 Mg m^{-3}, *T* = 173 K, *R* = 0.0345, R_W = 0.0801 for 4529 reflections with $I>2\sigma(I)$ and 395 variables. Data were collected using graphite monochromated Mo-Kα radiation, λ = 0.71075 Å.

2-(2-(Benzylsulfinyl)phenyl)-4,4-dimethyl-4,5-dihydrooxazole 17

A solution of sodium periodate (1.14 g, 5.33 mmol) in water (4 mL) was added dropwise to a stirred suspension of 2-(2-(benzylthio)phenyl)-4,4-dimethyl-4,5-dihydrooxazole **15** (1.49 g, 5.01 mmol) in methanol (10 mL). After stirring at rt for 18 h, the inorganic salts were removed by

filtration and washed with CH_2Cl_2 (3 × 25 mL). The combined filtrate was dried and evaporated and the crude residue was purified by column chromatography (SiO_2, Et_2O/hexane 7:3) to give, at R_f 0.55, **17** (0.50 g, 32%) as a colourless oil. IR: 2967, 1645, 1454, 1352, 1312, 1076, 1026, 962, 775, 741, 698 cm^{-1}. ^1H NMR (500 MHz): δ = 7.914 (dd, *J* = 7.8, 1.3 Hz, 1 H), 7.908 (dd, *J* = 7.8, 1.3 Hz, 1 H), 7.57 (td, *J* = 7.5, 1.0 Hz, 1 H), 7.49 (td, *J* = 7.5, 1.5 Hz, 1 H), 7.31–7.26 (m, 5 H), 4.62 (half AB pattern, *J* = 12.5 Hz, 1 H, S(O)CH_2), 4.13 and 4.11 (AB pattern, *J* = 8.0 Hz, 2 H, OCH_2) 3.93 (half AB pattern, *J* = 12.5 Hz, 1 H, S(O)CH_2), 1.47 (s, 3 H, CH_3), 1.41 (s, 3 H, CH_3). ^{13}C NMR (125 MHz): δ = 159.1 (C=N), 145.8 (C), 131.7 (C), 131.3 (CH), 130.1 (2 CH), 129.9 (CH), 129.0 (CH), 128.1 (2 CH), 127.8 (CH), 125.0 (CH), 124.8 (C), 78.8 (OCH_2), 68.8 (C), 61.9 (S(O)CH_2), 28.6 (CH_3), 28.4 (CH_3). HRMS ($ASAP^+$): *m/*z calcd for $C_{18}H_{20}NO_2S$ $[M+H]^+$: 314.1209; found: 314.1211.

2-Methyl-2-nitropropyl 2-(benzylsulfonyl)benzoate 19 and 2-(2-(Benzylsulfonyl)phenyl)-4,4-dimethyl-4,5-dihydrooxazole 18

A solution of mCPBA (50–55% purity, 3.45 g, 10.0–11.0 mmol) in CH_2Cl_2 (15 mL) was added dropwise to a stirred solution of 2-(2-(benzylthio)phenyl)-4,4-dimethyl-4,5-dihydrooxazole **15** (1.19 g, 4.00 mmol) in CH_2Cl_2 (15 mL). After stirring at rt for 18 h, the reaction mixture was washed with 2 M NaOH (3 × 30 mL) and water (30 mL) before being dried and evaporated. The crude residue was purified by column chromatography (SiO_2, Et_2O/hexane 3:2) to give, at R_f 0.65, **19** (0.44 g, 29%) as a colourless solid, mp 97–100 °C. IR: 2934, 1736, 1543, 1319, 1254, 1126, 1109, 1055, 887, 787, 762, 698 cm^{-1}. ^1H NMR (500 MHz): δ = 7.61–7.59 (m, 2 H), 7.52 (d, *J* = 8.0 Hz, 1 H), 7.44–7.39 (m, 1 H), 7.31–7.21 (m, 5 H), 4.77 (s, 2 H, CH_2), 4.74 (s, 2 H, CH_2), 1.73 (s, 6 H, CH_3). ^{13}C NMR (125 MHz): δ = 166.4 (C=O), 136.7 (C), 133.4 (CH), 132.3 (C), 131.5 (CH), 131.0 (2 CH), 130.8 (CH), 129.3 (CH), 128.7 (CH), 128.5 (2 CH), 127.9 (C), 86.2 (CNO_2), 69.5 (CH_2), 62.7 (CH_2), 23.2 (CH_3). HRMS (NSI^+): *m/*z calcd for $C_{18}H_{23}N_2O_6S$ $[M+NH_4]^+$: 395.1271; found: 395.1271.

This was followed by a second fraction at R_f 0.50 to give **18** (0.74 g, 56%) as colourless crystals, mp 138–141 °C. IR: 2970, 1670, 1314, 1252, 1165, 1123, 1094, 1047, 955, 926, 895, 793, 772, 700 cm^{-1}. ^1H NMR (500 MHz): δ = 7.71 (dd, *J* = 7.5, 1.0 Hz, 1 H), 7.59 (td, *J* = 7.5, 1.5 Hz, 1 H), 7.56 (dd, *J* = 8.0, 1.0 Hz, 1 H), 7.38 (td, *J* = 7.8, 1.0 Hz, 1 H), 7.30–7.22 (m, 5 H), 4.82 (s, 2 H, SO_2CH_2), 4.25 s, (2 H, OCH_2), 1.48 (s, 6 H, CH_3). ^{13}C NMR (125 MHz): δ = 160.8 (C=N), 137.2 (C), 133.2 (CH), 131.3 (CH), 131.0 (2 CH), 130.8 (CH), 130.0 (CH), 129.6 (C), 128.5 (CH), 128.4 (2 CH), 128.3 (C), 79.9 (OCH_2), 68.5 (C), 62.4 (SO_2CH_2), 27.9 (CH_3). HRMS (NSI^+): *m/*z calcd for $C_{18}H_{20}NO_3S$ $[M+H^+]$: 330.1158; found: 330.1154.

4',4'-Dimethyl-2-phenyl-2*H*-spiro[benzo[*b*]thiophene-3,2'-oxazolidine] *S*,*S*-dioxide 20

The same procedure as for **3** using *n*-butyllithium (0.50 mL, 1.25 mmol), 2-(2-(benzylsulfonyl)phenyl)-4,4-dimethyl-4,5-dihydrooxazole **18** (0.1657 g, 0.50 mmol) and potassium *tert*-butoxide (0.1428 g, 1.27 mmol) in dry THF (5 mL) gave, after purification by preparative TLC (SiO_2, Et_2O/hexane 7:3), at R_f 0.15, **20** (0.1089 g, 66%) as pale yellow crystals, mp 138–142 °C. IR: 3333, 2972, 2891, 1452, 1294, 1150, 1132, 1047, 760, 729, 700, 615, 565 cm^{-1}. ^1H NMR showed a 3:2 mixture of diastereomers. ^1H NMR (400 MHz, major diastereomer): δ = 7.85–7.37 (m, 9 H), 4.70 (s, 1 H, SO_2CHPh), 3.78 and 3.41 (AB pattern, *J* = 8.3 Hz, 2 H, CH_2), 2.35 (br s, 1 H, NH), 1.31 (s, 3 H, CH_3), 0.78 (s, 3 H, CH_3). ^{13}C NMR (125 MHz, major diastereomer): δ = 142.5 (C), 139.2 (C), 134.0 (CH), 131.6 (2 CH), 130.71 (CH), 129.22 (CH), 128.4 (2 CH), 127.5 (C),

124.6 (CH), 121.4 (CH), 98.5 (spiro C), 78.9 (CH_2), 75.6 (SO_2CHPh), 59.6 (C), 28.5 (CH_3), 26.4 (CH_3). ^{1}H NMR (400 MHz, minor diastereomer): δ = 7.85–7.37 (m, 9 H), 4.52 (s, 1 H, SO_2CHPh), 3.62 and 3.29 (AB pattern, *J* = 8.3 Hz, 2 H, CH_2), 2.35 (br s, 1 H, NH), 1.37 (s, 3 H, CH_3), 0.83 (s, 3 H, CH_3). ^{13}C NMR (125 MHz, minor diastereomer): δ = 141.8 (C), 139.1 (C), 133.8 (CH), 132.0 (2 CH), 130.73 (CH), 129.19 (CH), 129.1 (C), 128.2 (2 CH), 124.5 (CH), 121.6 (CH), 97.8 (spiro C), 78.6 (CH_2), 75.4 (SO_2CHPh), 58.5 (C), 27.6 (CH_3), 27.0 (CH_3). HRMS (NSI^+): *m/*z calcd for $C_{18}H_{20}NO_3S$ $[M+H^+]$: 330.1158; found: 330.1151.

_N_-Benzyl-2-(4,4-dimethyl-4,5-dihydrooxazol-2-yl)-_N_-methylaniline 21

A literature procedure[14] was adapted as follows: under a nitrogen atmosphere, *n*-butyllithium (2.5 M in hexane, 4.0 mL, 10.0 mmol) was added dropwise to a stirred –78 °C solution of *N*-benzylmethylamine (1.3 mL, 1.22 g, 10.1 mmol) in dry THF (15 mL). Once the addition was complete, the reaction mixture was allowed to warm to 0 °C for 30 min before a solution of 2-(2-methoxyphenyl)-4,4-dimethyl-4,5-dihydrooxazole[15] (2.06 g, 10.0 mmol) in dry THF (20 mL) was added dropwise. The reaction mixture was allowed to warm to rt over 18 h before being quenched by addition of water (4 mL) and concentrated at reduced pressure. The residue was partitioned between Et_2O (100 mL) and water (100 mL), the two layers were separated and the aqueous layer re-extracted with Et_2O (2 × 50 mL). The combined organic layers were washed with sat aq. Na_2CO_3 (100 mL) before being dried and evaporated. The crude residue was purified by column chromatography (SiO_2, Et_2O/hexane 7:3) to give, at R_f 0.35, **21** (1.60 g, 54%) as a yellow oil. IR: 2965, 1646, 1598, 1495, 1452, 1364, 1310, 1100, 1037, 965, 871, 758, 699 cm^{-1}. ^{1}H NMR (500 MHz): δ = 7.61 (dd, *J* = 7.5, 1.5 Hz, 1 H), 7.33–7.28 (m, 5 H), 7.26–7.22 (m, 1 H), 6.95 (d, *J* = 8.5 Hz, 1 H), 6.92 (t, *J* = 7.5 Hz, 1 H), 4.30 (s, 2 H, CH_2), 3.98 (s, 2 H, CH_2), 2.74 (s, 3 H, NCH_3), 1.31 (s, 6 H, CH_3). ^{13}C NMR (75 MHz): δ = 164.0 (C=N), 151.5 (C), 138.2 (C), 132.0 (CH), 131.2 (CH), 128.2 (2 CH), 127.8 (2 CH), 126.9 (CH), 120.3 (C), 120.1 (CH), 118.2 (CH), 79.1 (OCH_2), 67.0 (C), 60.1 (NCH_2), 39.7 (NCH_3), 28.3 (CH_3). HRMS (ESI^+): *m/*z calcd for $C_{19}H_{23}N_2O$ $[M+H]^+$: 295.1805; found: 295.1796.

2-Methyl-2-((1-methyl-2-phenyl-1*H*-indol-3-yl)amino)propan-1-ol 22

The same procedure as for **3** using *n*-butyllithium (4.0 mL, 10.0 mmol), *N*-benzyl-2-(4,4-dimethyl-4,5-dihydrooxazol-2-yl)-*N*-methylaniline **21** (1.18 g, 4.01 mmol) and potassium *tert*-butoxide (1.14 g, 10.2 mmol) in dry THF (40 mL) gave, after purification by column chromatography (SiO_2, Et_2O/hexane 7:3) a 2:1 mixture of **22** and **21**. Rechromatography (Al_2O_3, Et_2O/hexane 7:3) of this gave, at R_f 0.55, **22** (0.43 g, 36%) as tan-coloured crystals, mp 102–106 °C. IR: 3283, 2959, 1470, 1360, 1327, 1246, 1155, 1072, 1049, 1024, 741, 700 cm^{-1}. ^{1}H NMR (400 MHz): δ = 7.69 (d, *J* = 7.6 Hz, 1 H), 7.50–7.45 (m, 2 H), 7.42–7.38 (m, 3 H), 7.30 (d, *J* = 8.0 Hz, 1 H), 7.24–7.20 (m, 1 H), 7.15–7.11 (m, 1 H), 3.56 (s, 3 H, NCH_3), 3.13 (s, 2 H, CH_2), 2.71 (br s, 2 H, NH and OH), 0.86 (s, 6 H, CH_3). ^{13}C NMR (100 MHz): δ = 135.6 (C), 135.5 (C), 131.6 (C), 130.5 (2 CH), 128.6 (2 CH), 128.1 (CH), 126.6 (C), 121.7 (CH), 119.3 (CH), 119.0 (CH), 118.2 (C), 109.1 (CH), 69.6 (CH_2), 57.6 (C), 30.8 (NCH_3), 24.8 (CH_3). HRMS (NSI^+): *m/*z calcd for $C_{19}H_{23}N_2O$ $[M+H]^+$: 295.1805; found: 295.1804.

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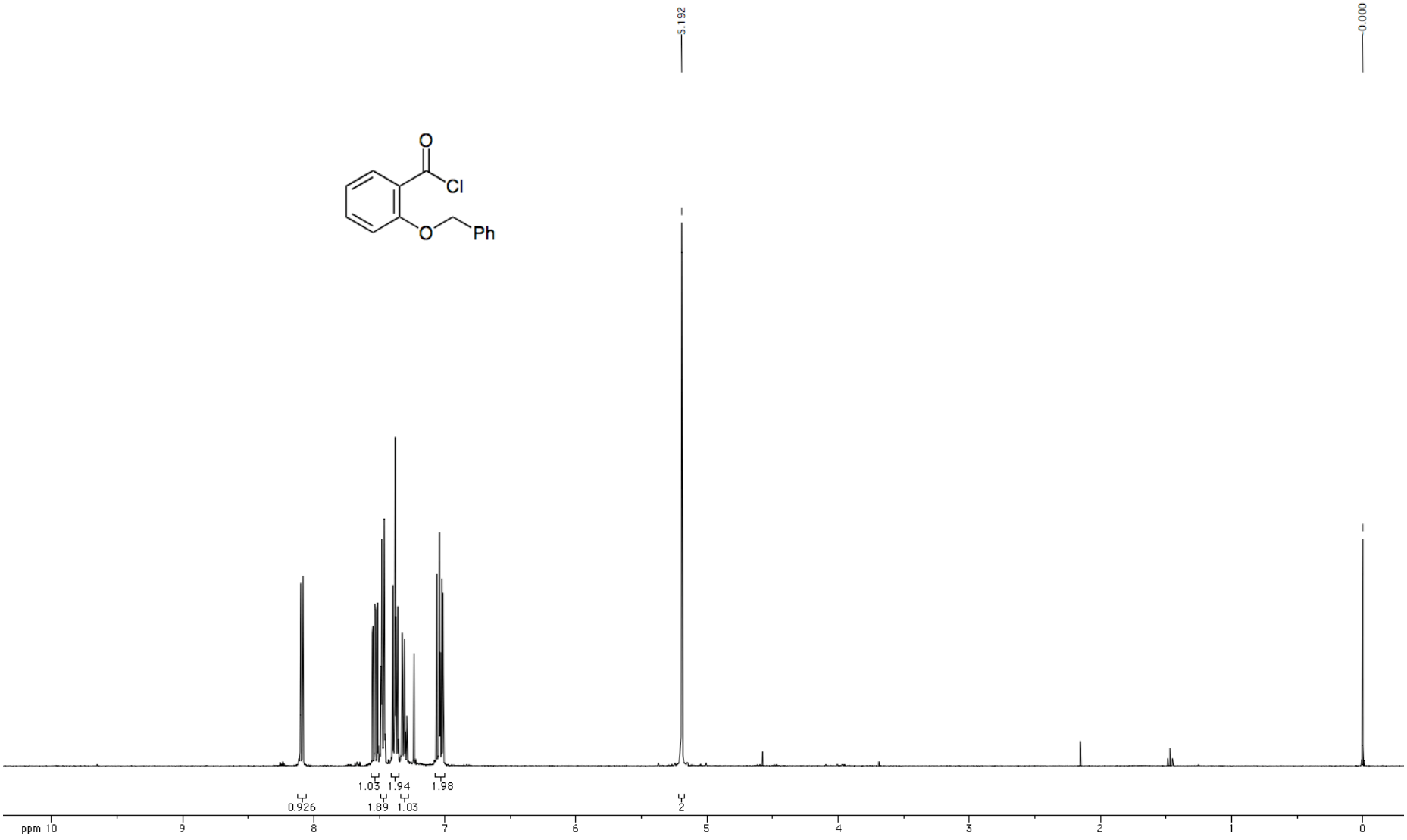
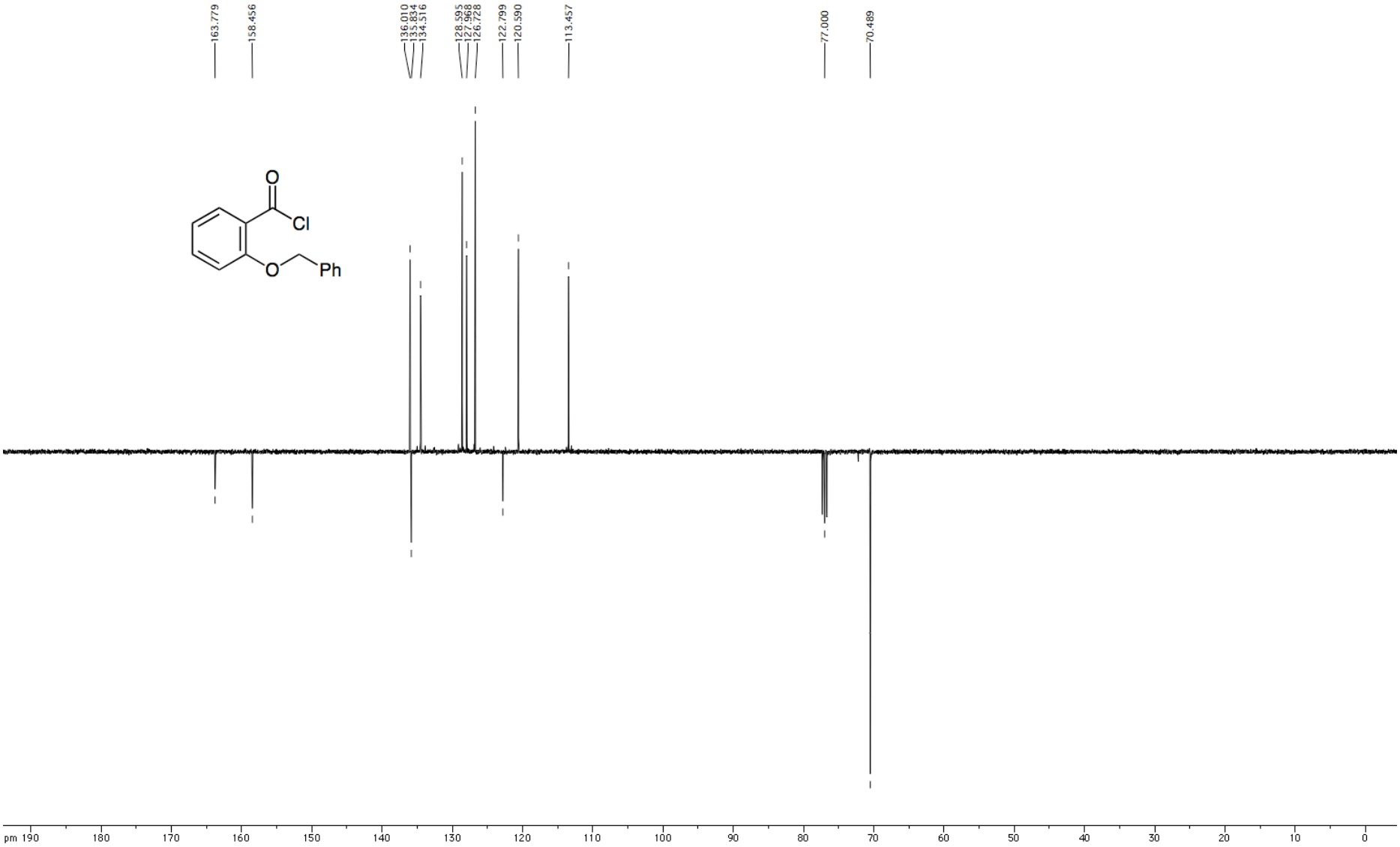
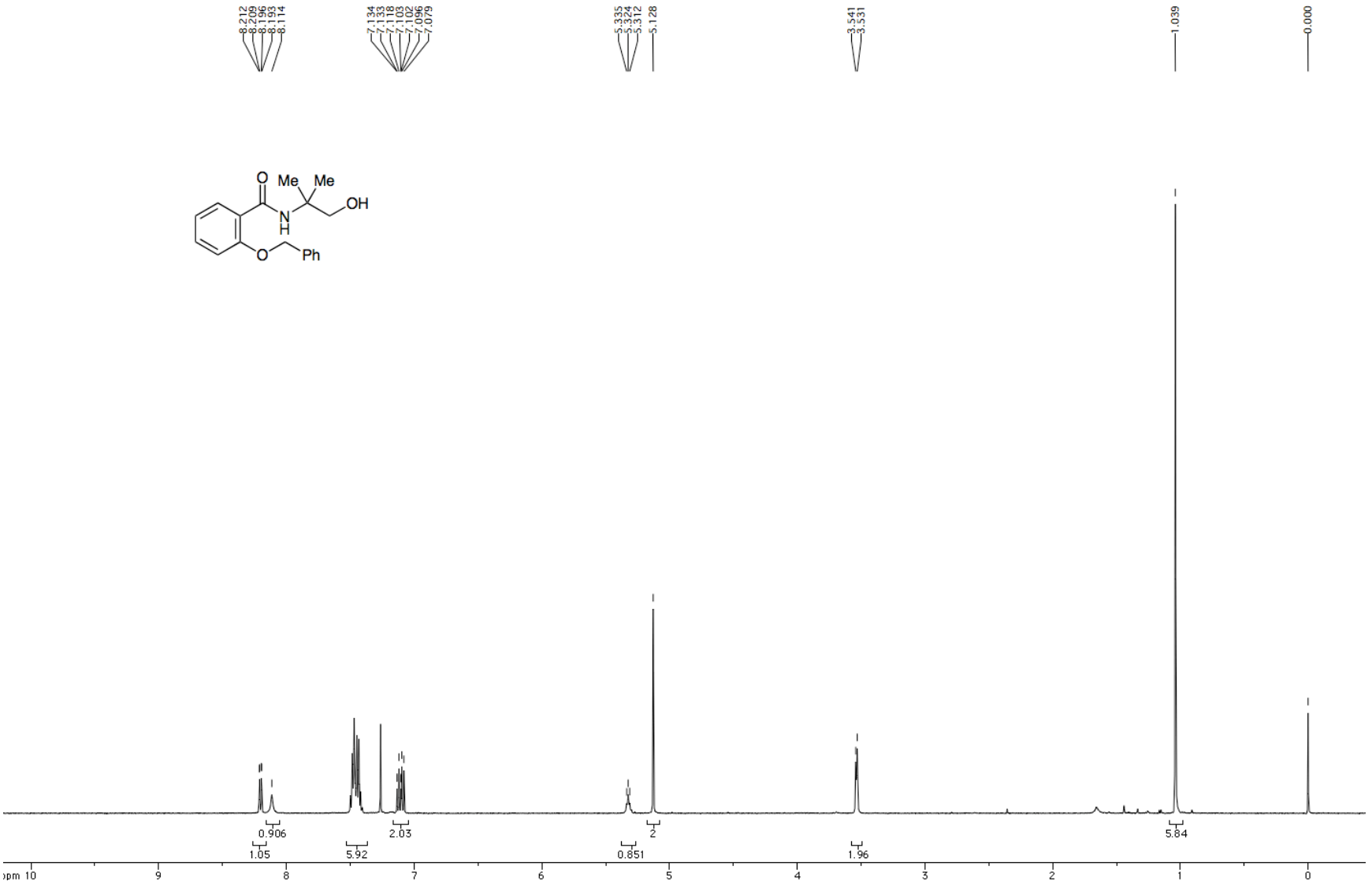
400 MHz ^{1}H NMR Spectrum of 2-(Benzyloxy)benzoyl chloride A



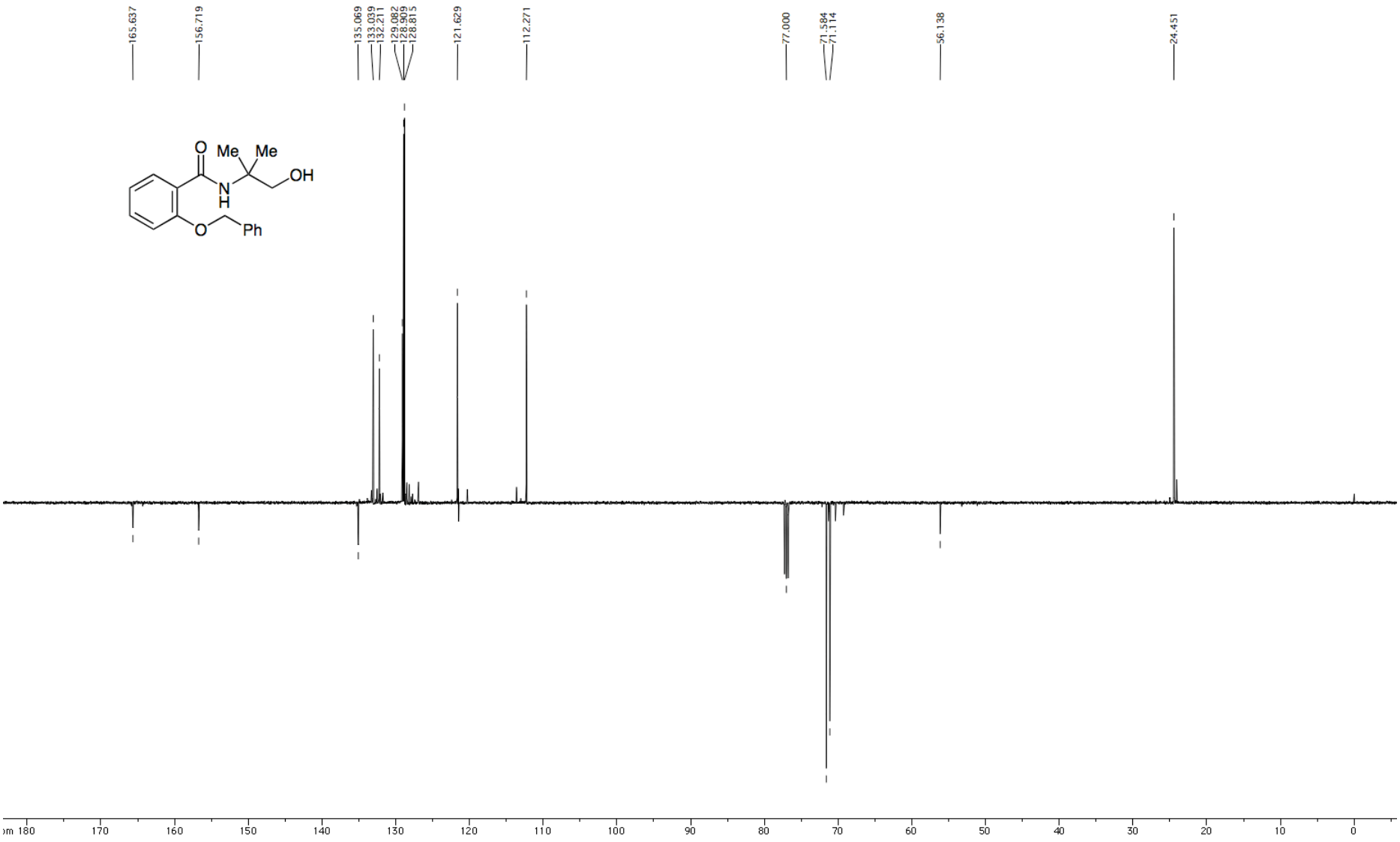
100 MHz DEPTQ ^{13}C NMR Spectrum of 2-(Benzyloxy)benzoyl chloride A



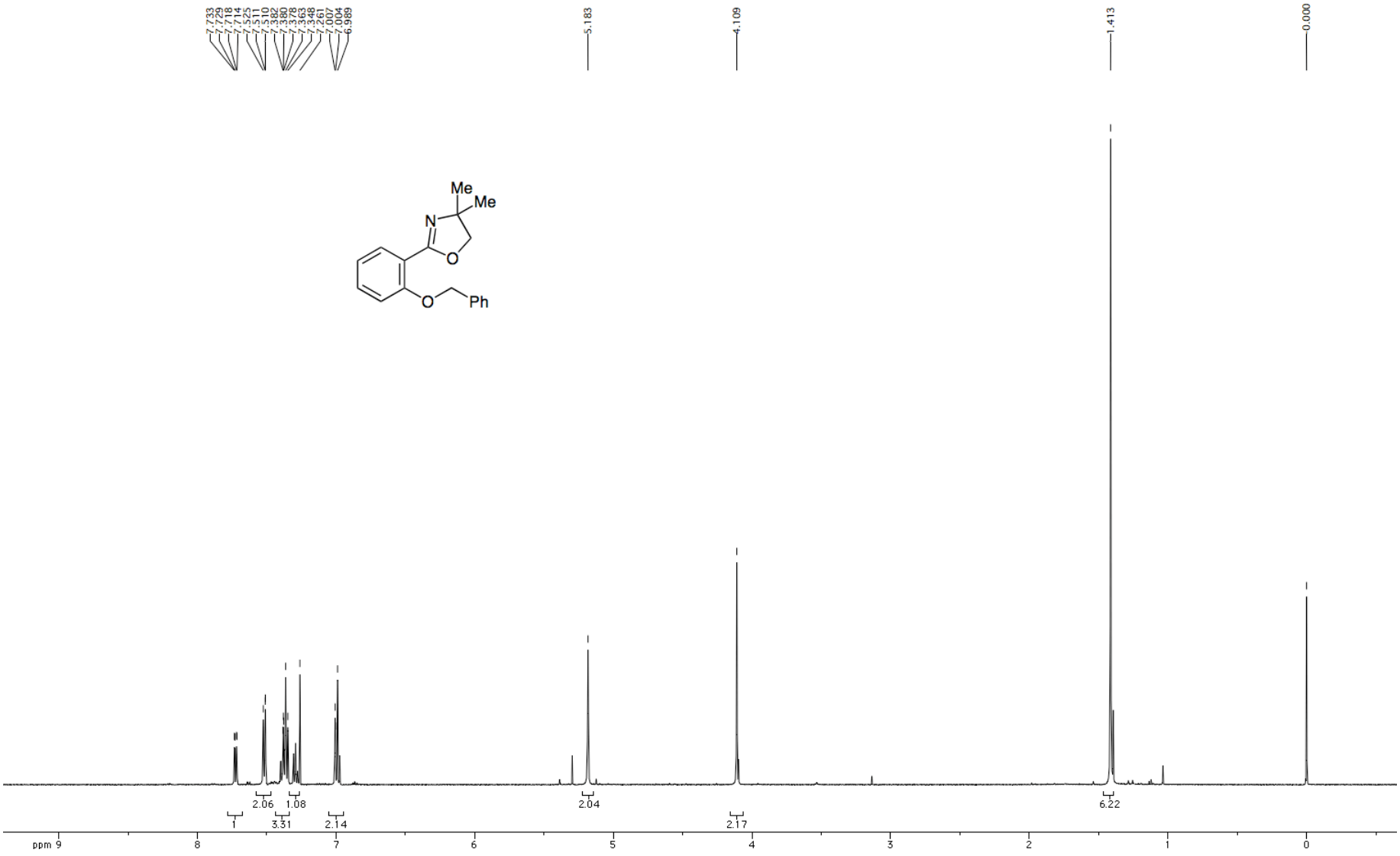
500 MHz ^{1}H NMR Spectrum of 2-(Benzyloxy)-*N*-(1-hydroxy-2-methylpropan-2-yl)benzamide B



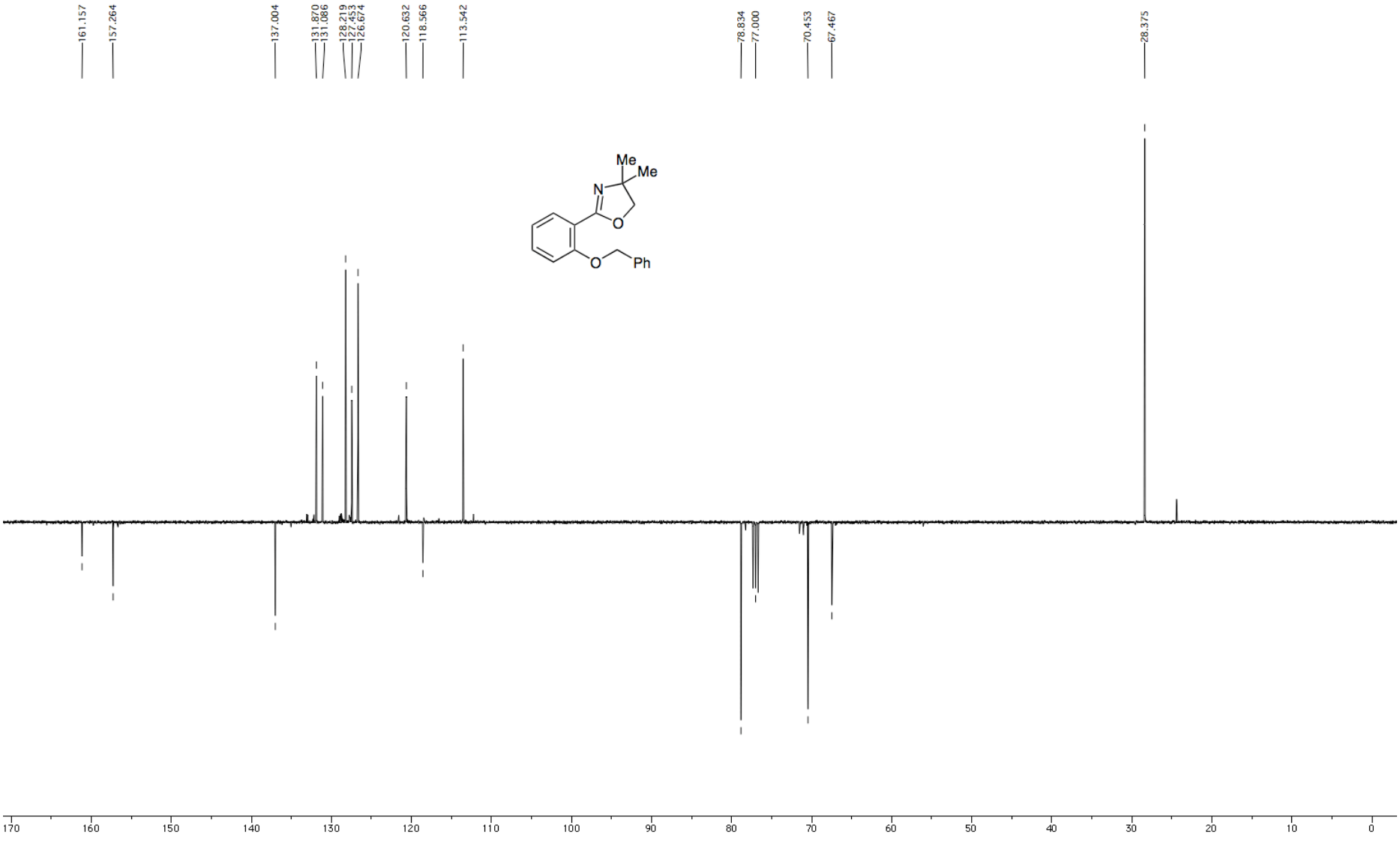
125 MHz DEPTQ ^{13}C NMR Spectrum of 2-(Benzyloxy)-*N*-(1-hydroxy-2-methylpropan-2-yl)benzamide B



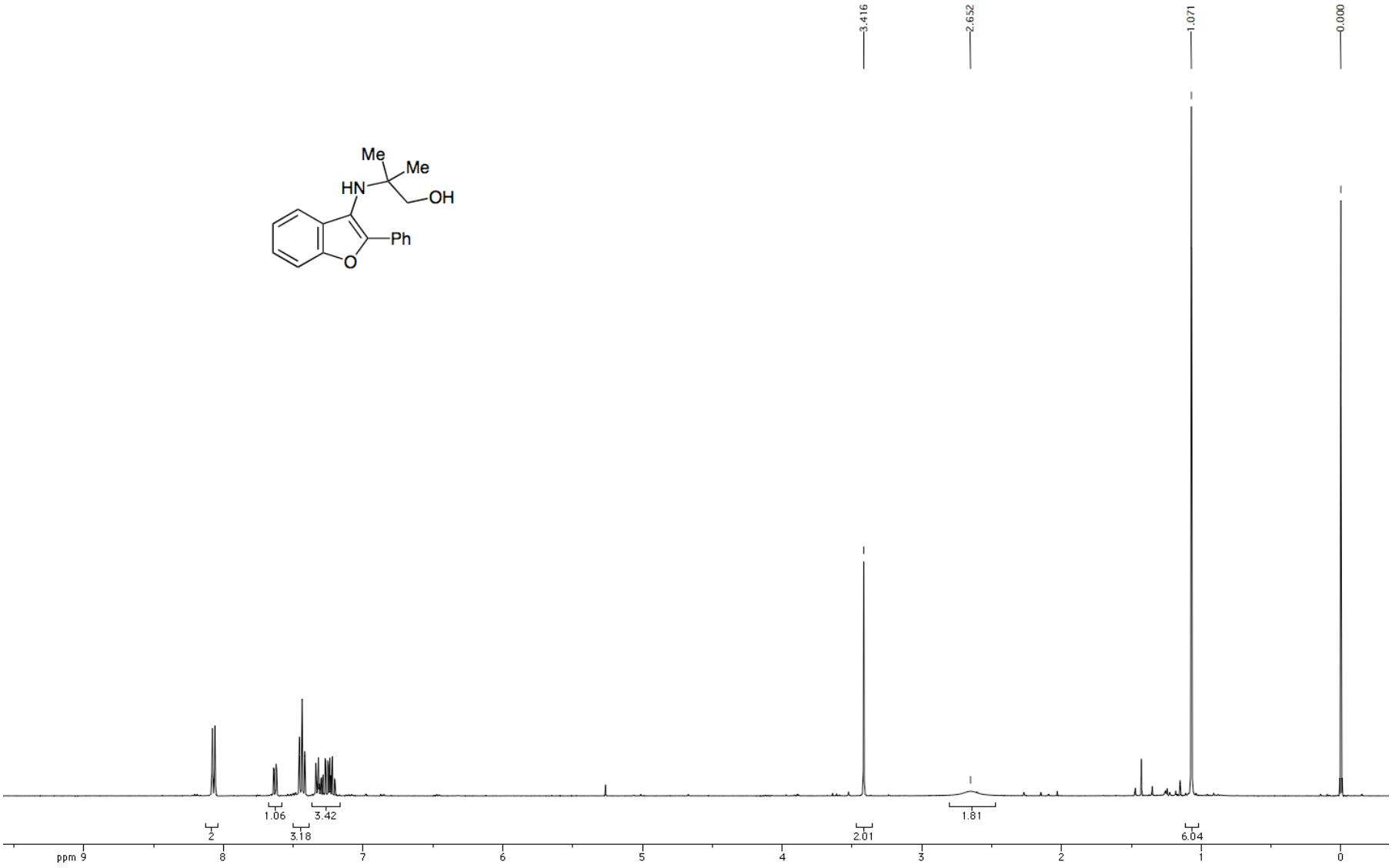
500 MHz ^{1}H NMR Spectrum of 2-(2-(Benzyloxy)phenyl)-4,4-dimethyl-4,5-dihydrooxazole 1



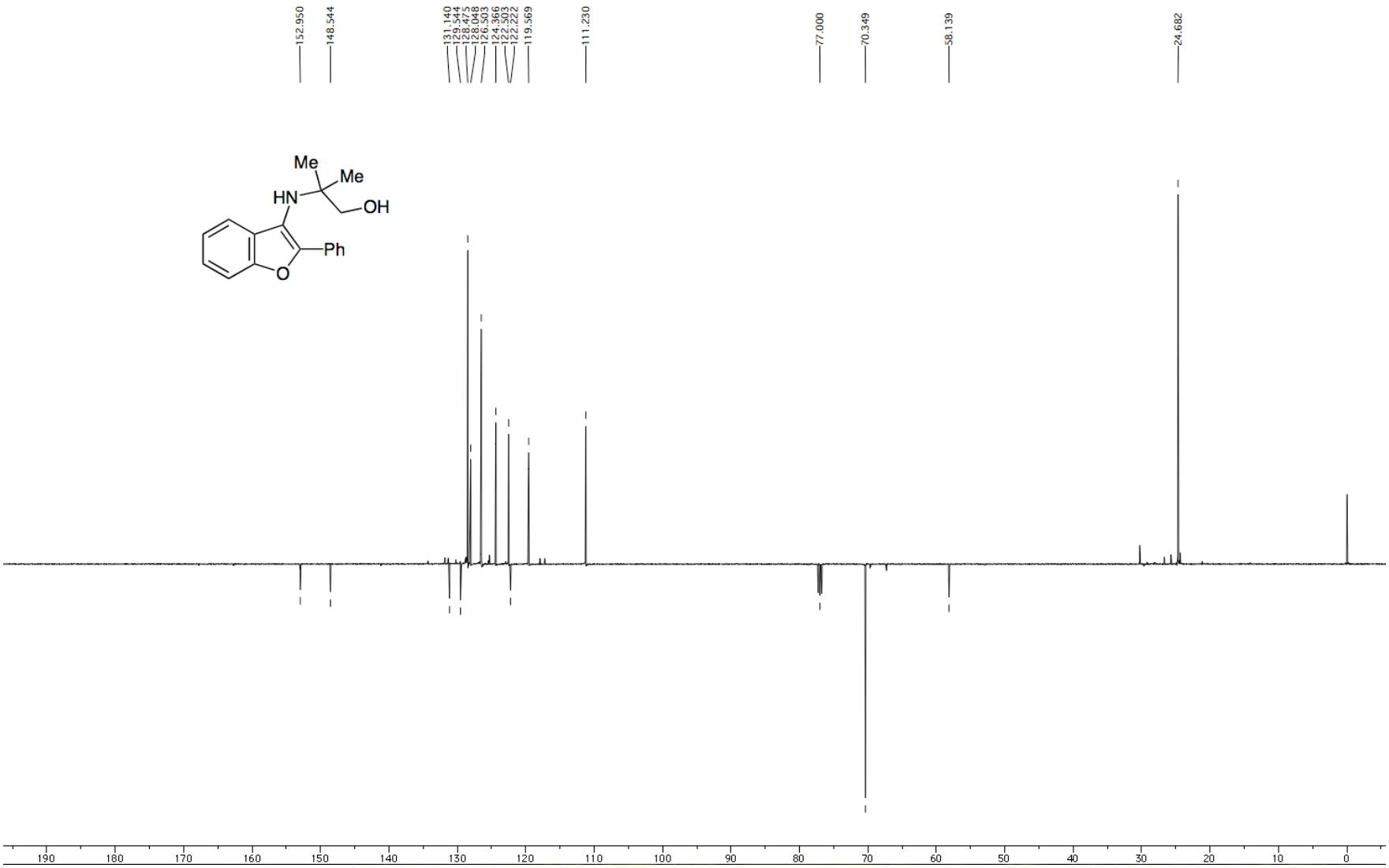
100 MHz DEPTQ ^{13}C NMR Spectrum of 2-(2-(Benzyloxy)phenyl)-4,4-dimethyl-4,5-dihydrooxazole 1



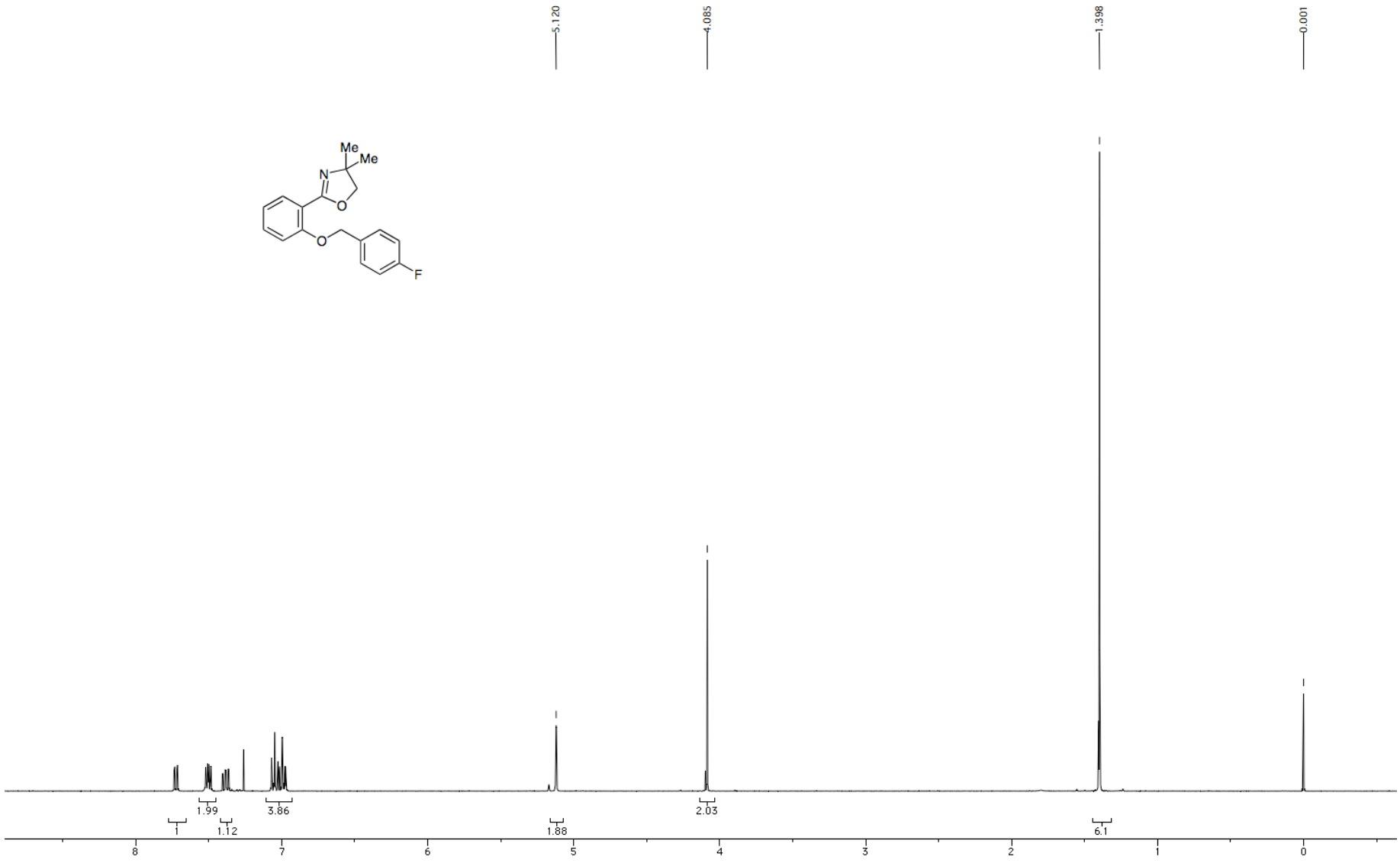
400 MHz ^{1}H NMR Spectrum of 2-Methyl-2-((2-phenylbenzofuran-3-yl)amino)propan-1-ol 3



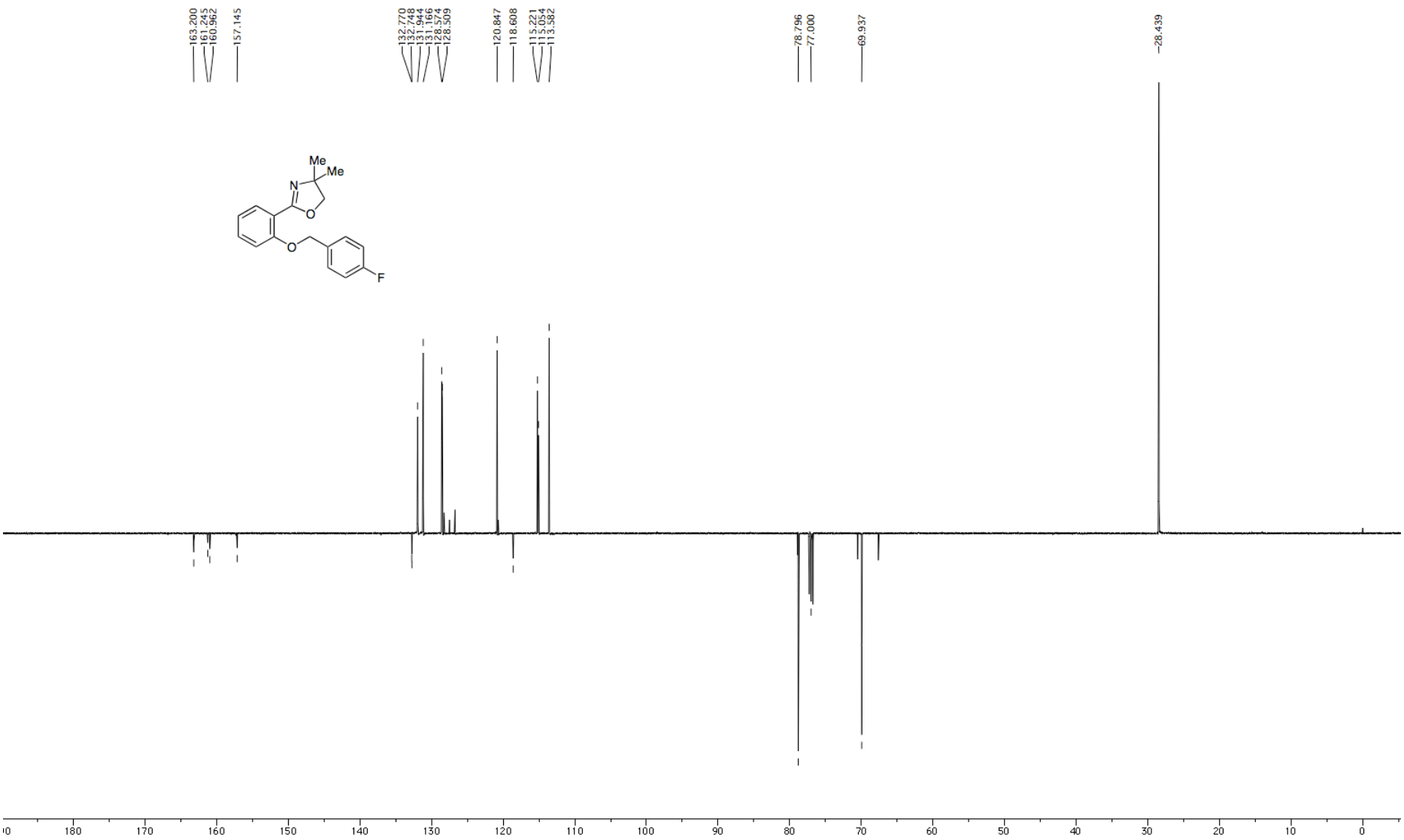
125 MHz DEPTQ ^{13}C NMR Spectrum of 2-Methyl-2-((2-phenylbenzofuran-3-yl)amino)propan-1-ol 3



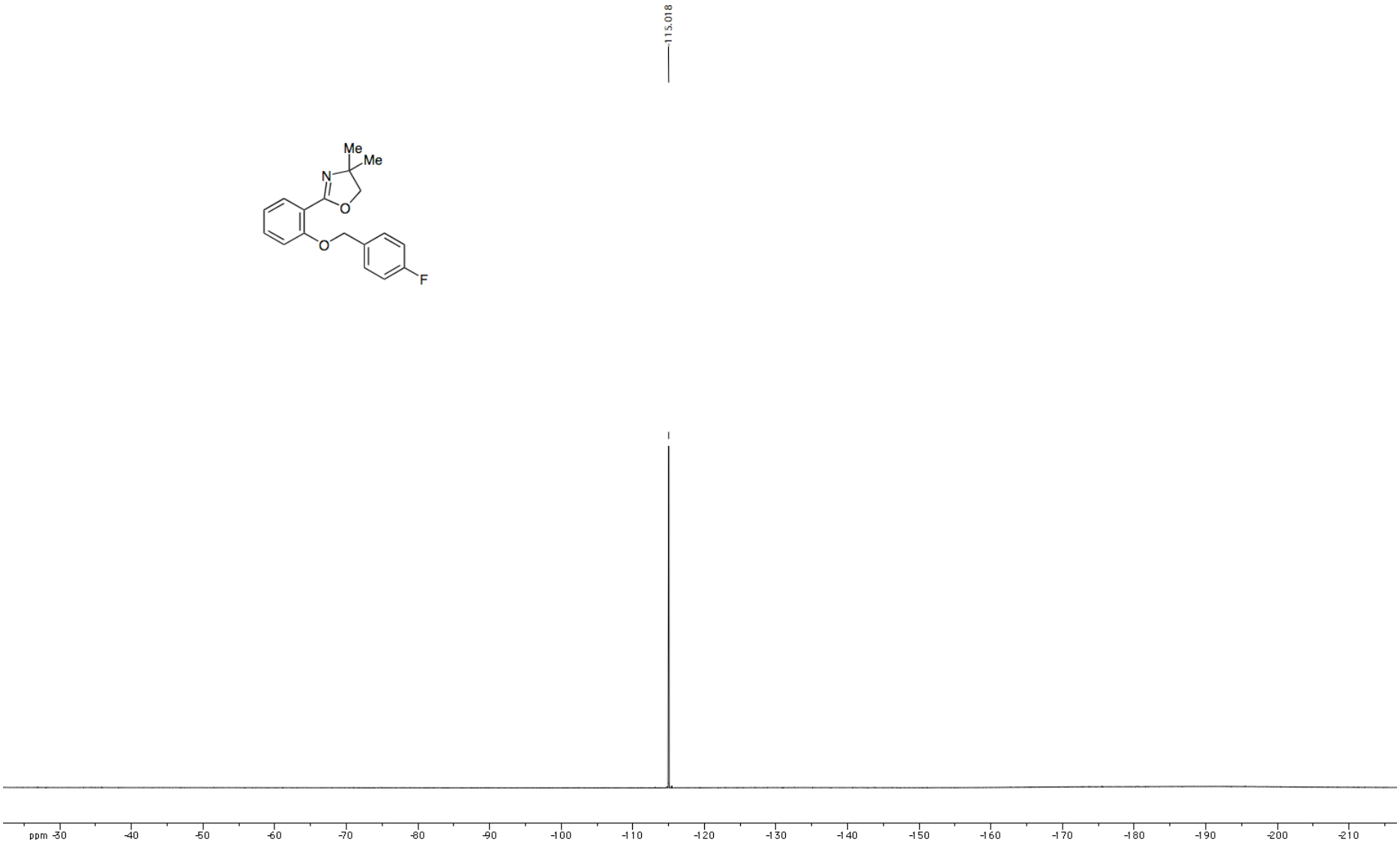
400 MHz ^{1}H NMR Spectrum of 2-(2-((4-Fluorobenzyl)oxy)phenyl)-4,4-dimethyl-4,5-dihydrooxazole 5a



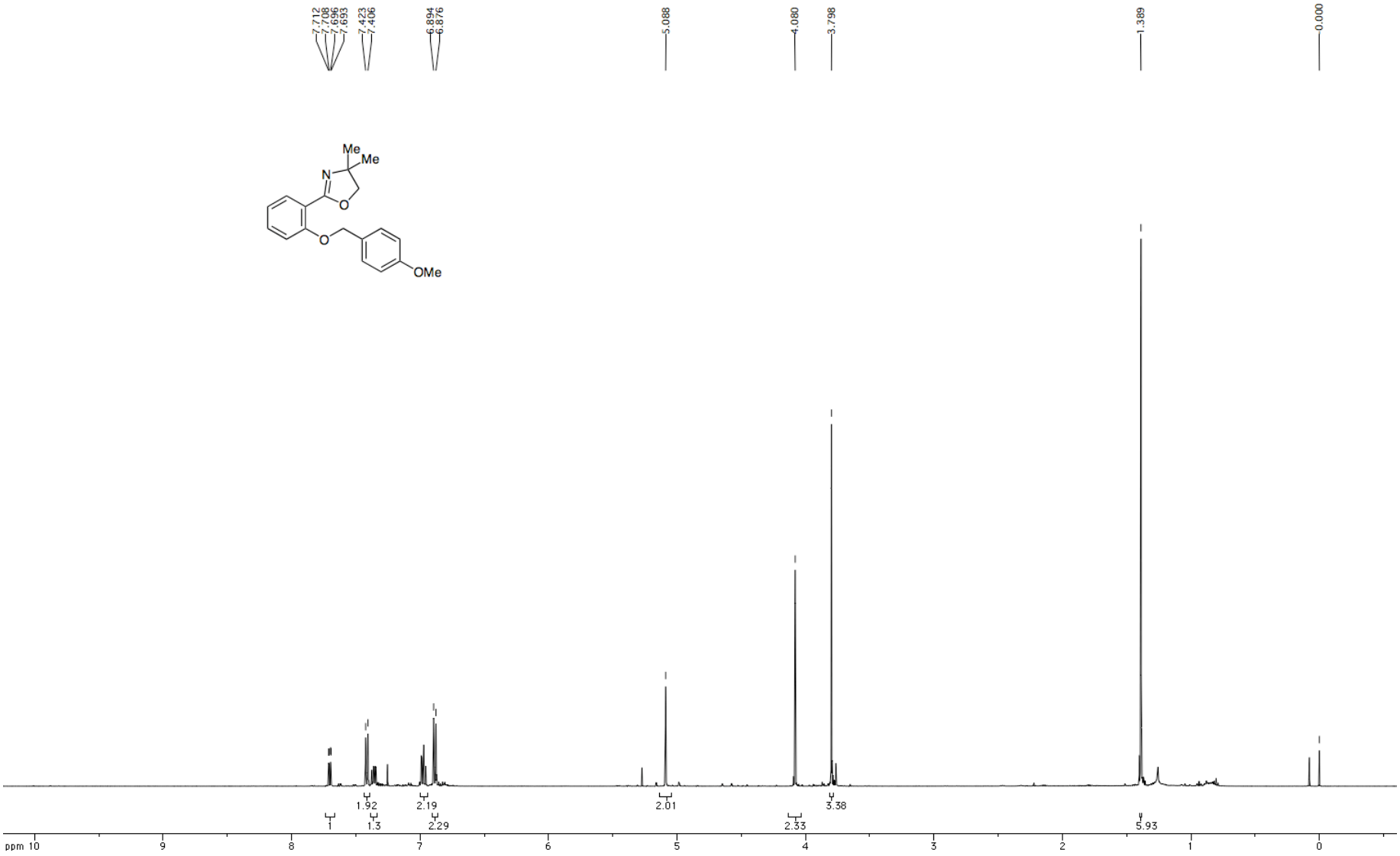
125 MHz DEPTQ ^{13}C NMR Spectrum of 2-(2-((4-Fluorobenzyl)oxy)phenyl)-4,4-dimethyl-4,5-dihydrooxazole 5a



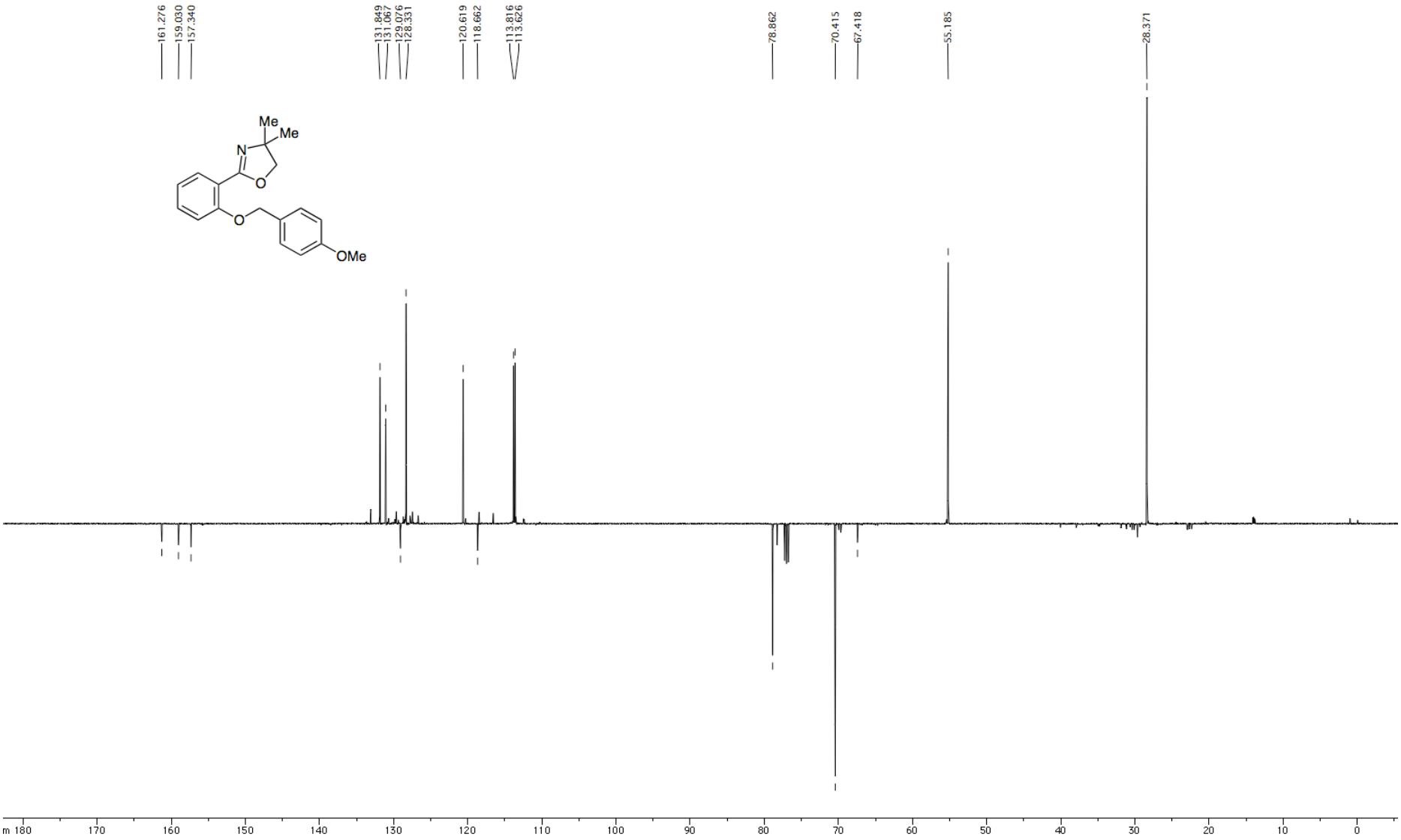
376 MHz ^{19}F NMR Spectrum of 2-(2-((4-Fluorobenzyl)oxy)phenyl)-4,4-dimethyl-4,5-dihydrooxazole 5a



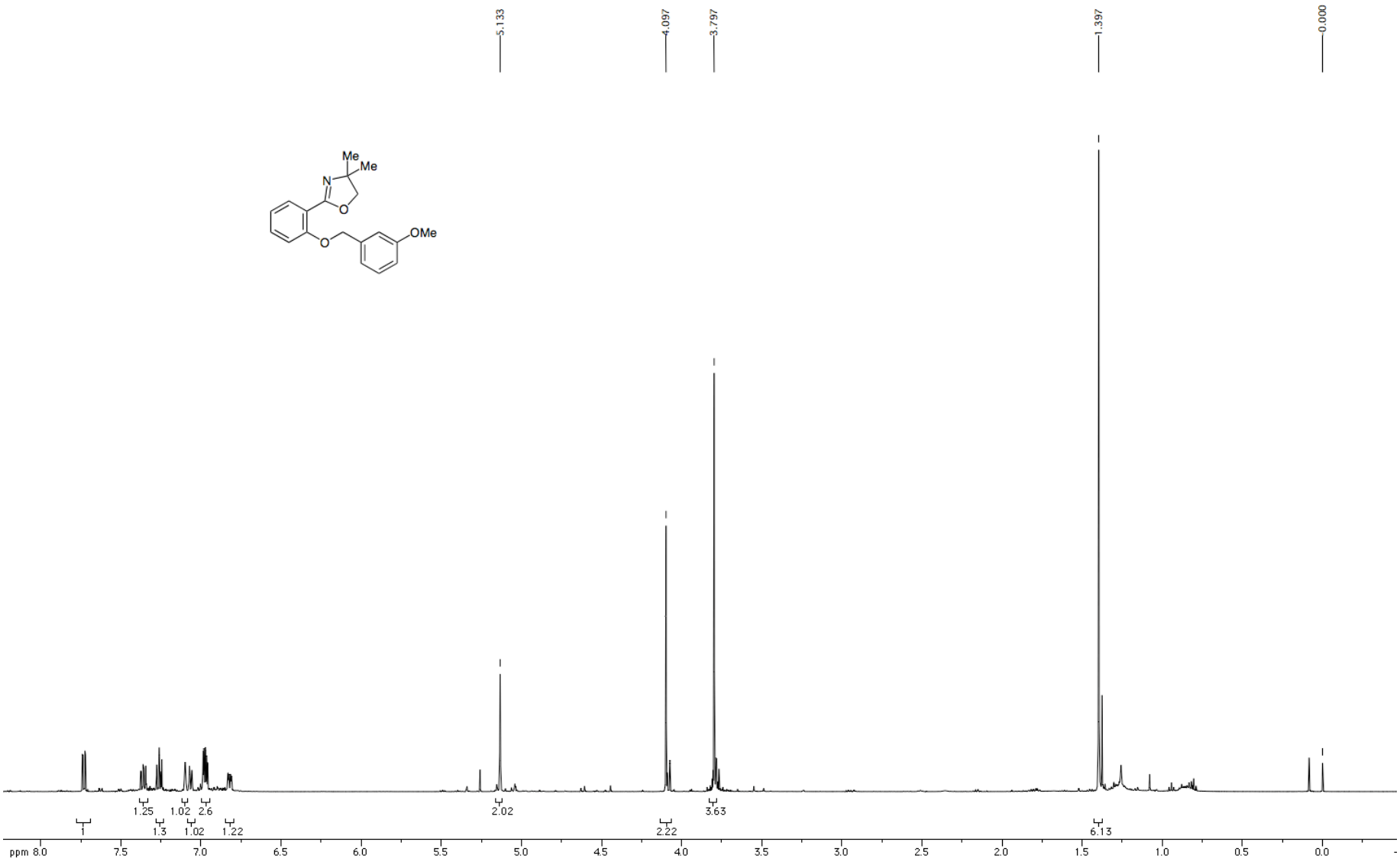
500 MHz ^{1}H NMR Spectrum of 2-(2-((4-Methoxybenzyl)oxy)phenyl)-4,4-dimethyl-4,5-dihydrooxazole 5b



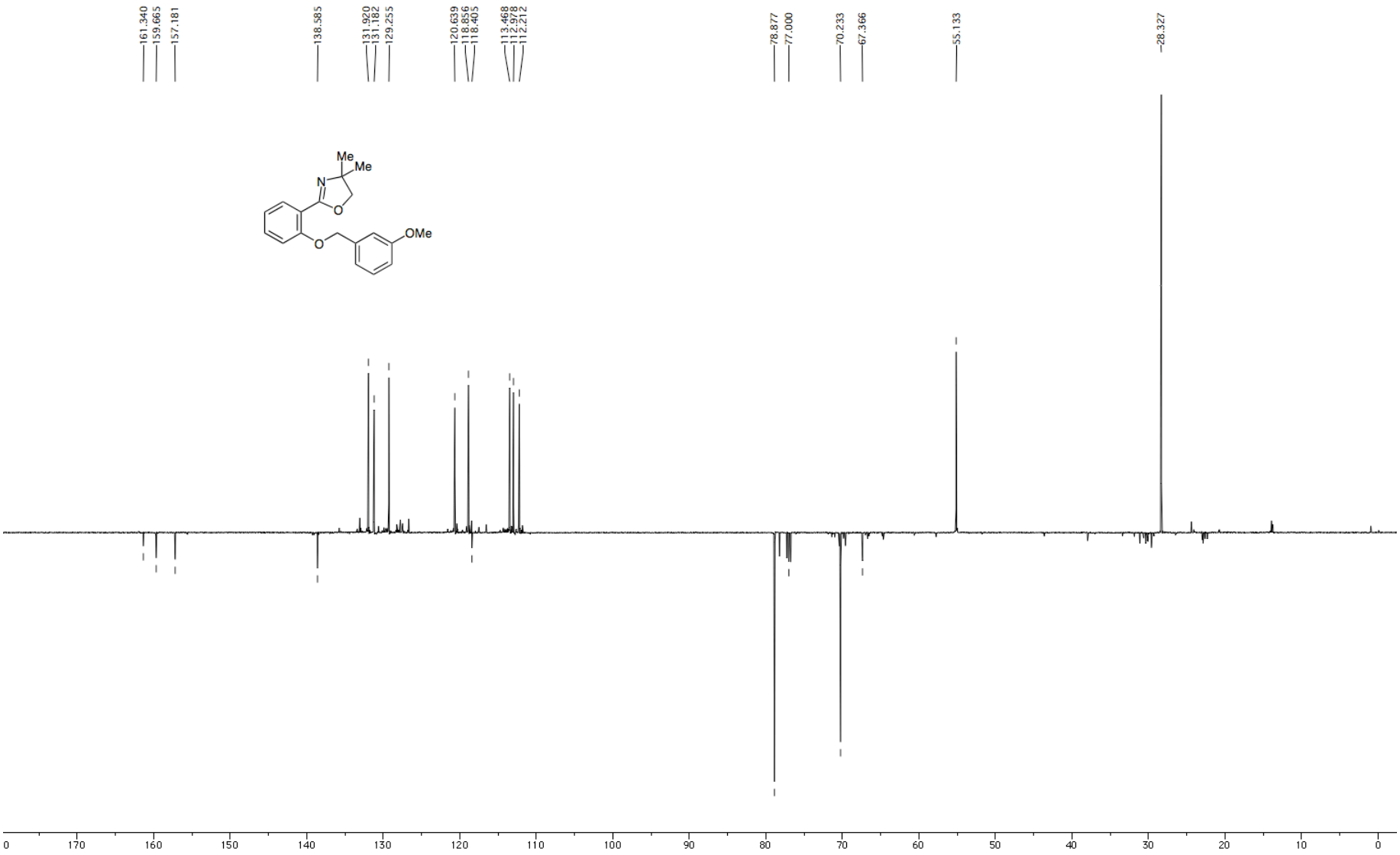
125 MHz DEPTQ ^{13}C NMR Spectrum of 2-(2-((4-Methoxybenzyl)oxy)phenyl)-4,4-dimethyl-4,5-dihydrooxazole 5b



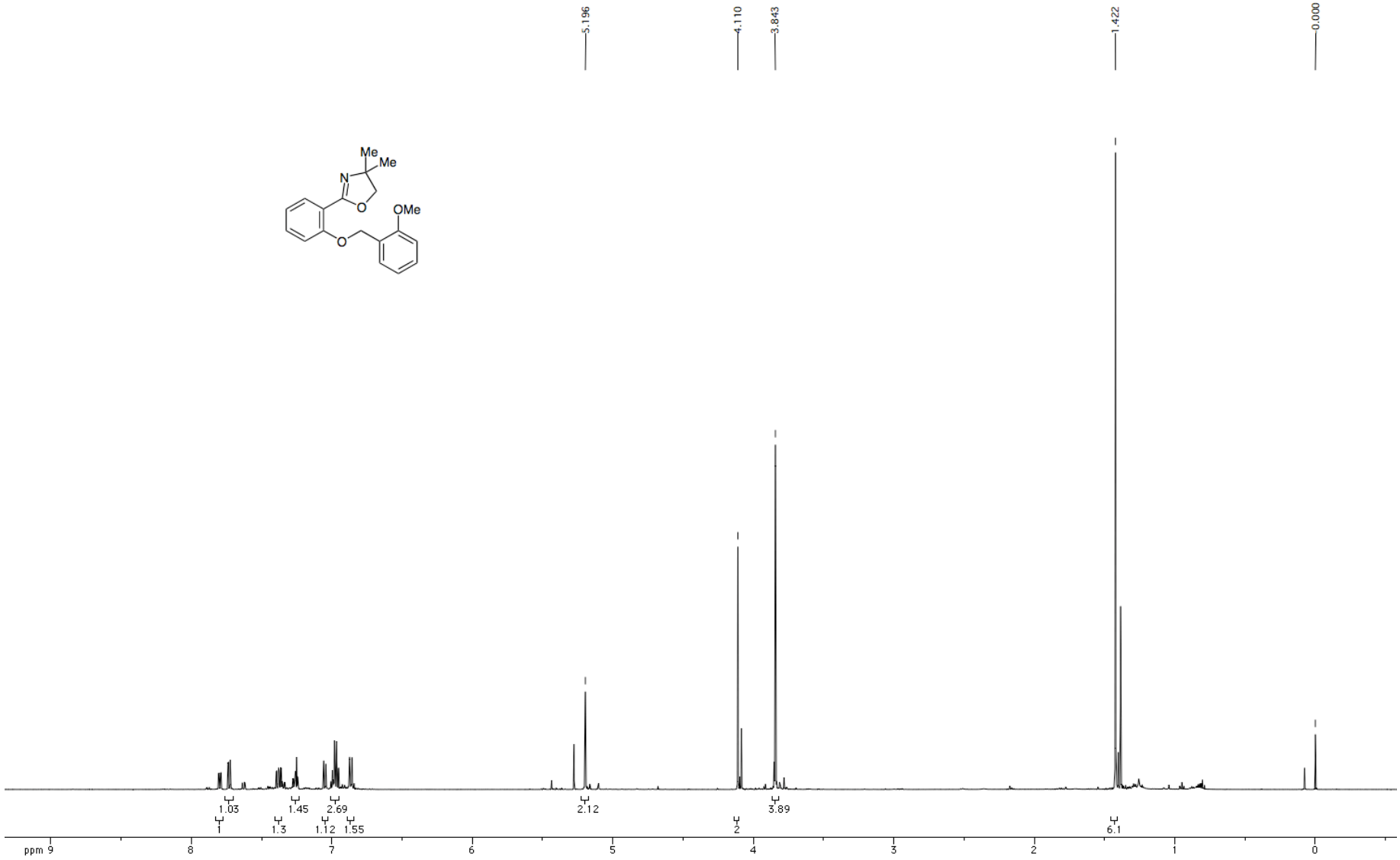
500 MHz ^{1}H NMR Spectrum of 2-(2-((3-Methoxybenzyl)oxy)phenyl)-4,4-dimethyl-4,5-dihydrooxazole 5c



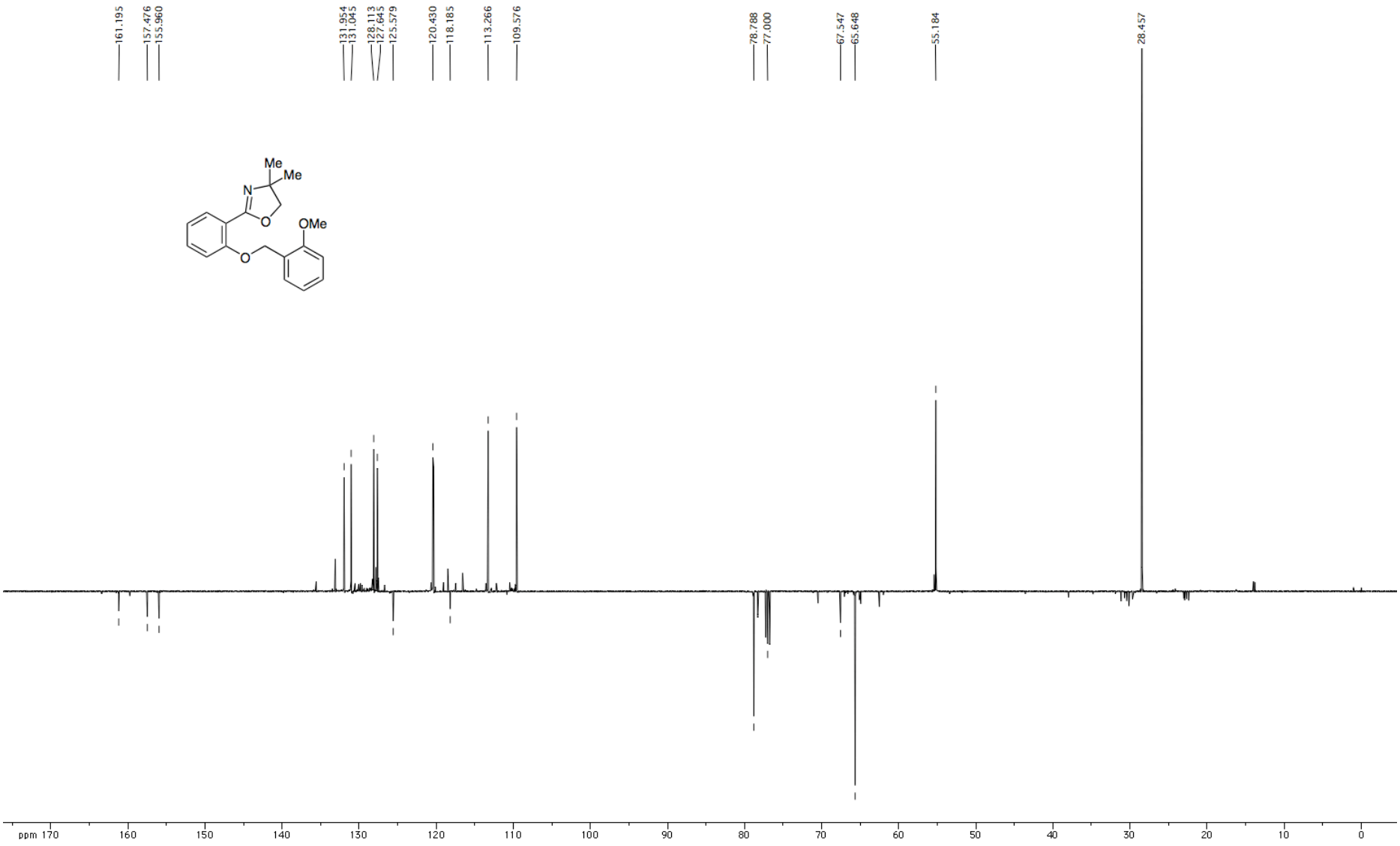
125 MHz DEPTQ ^{13}C NMR Spectrum of 2-(2-((3-Methoxybenzyl)oxy)phenyl)-4,4-dimethyl-4,5-dihydrooxazole 5c



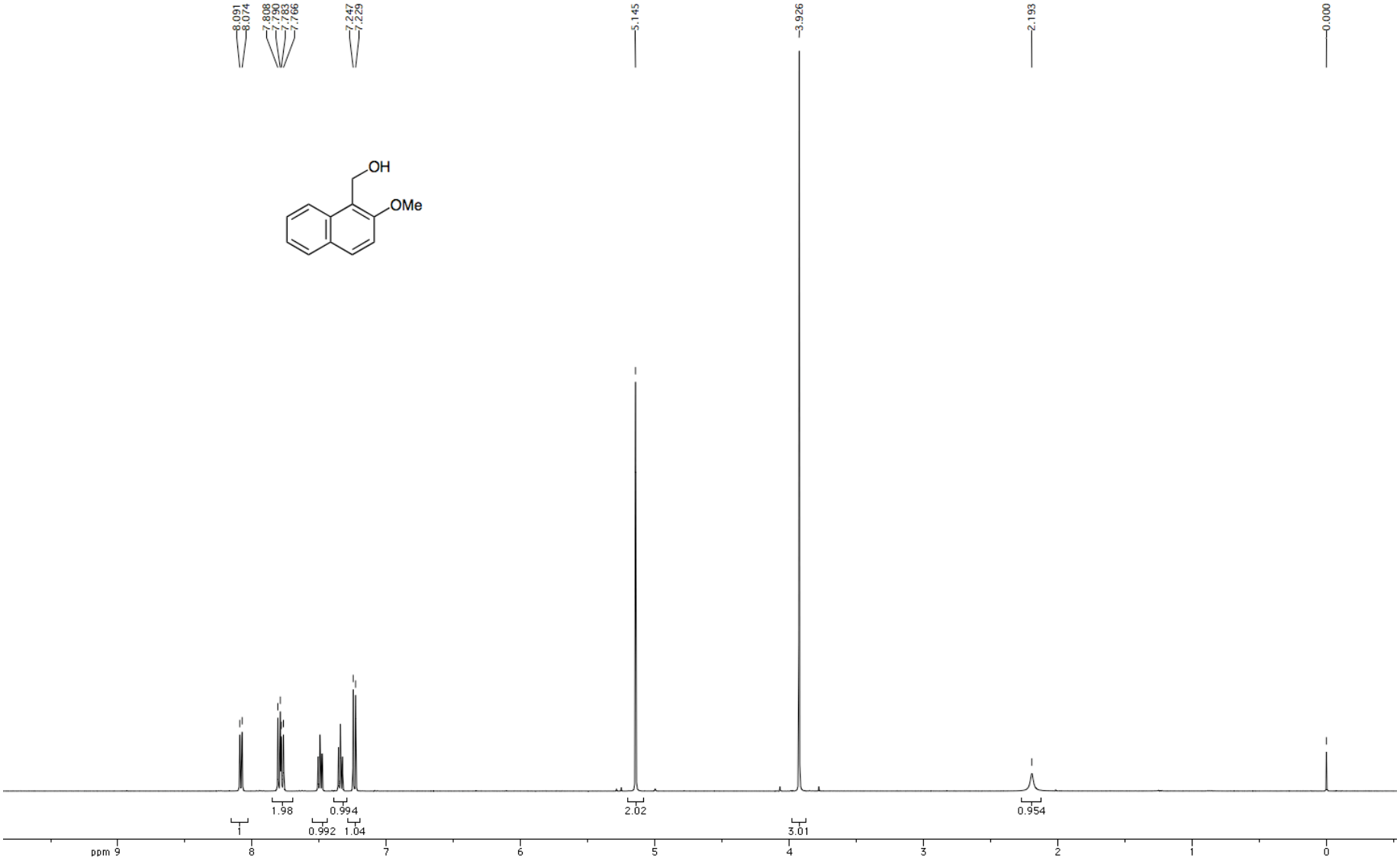
500 MHz ^{1}H NMR Spectrum of 2-(2-((2-Methoxybenzyl)oxy)phenyl)-4,4-dimethyl-4,5-dihydrooxazole 5d



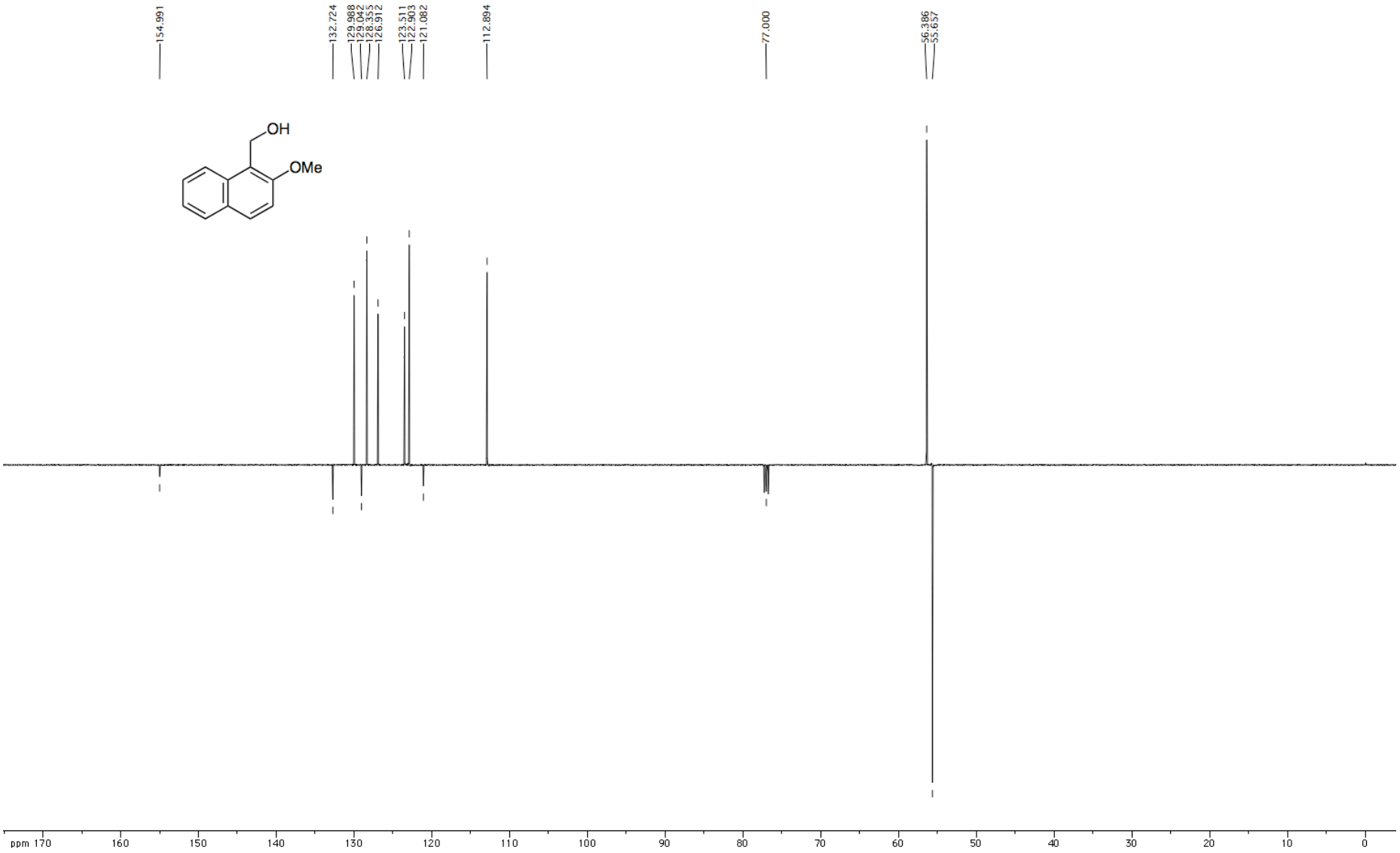
125 MHz DEPTQ ^{13}C NMR Spectrum of 2-(2-((2-Methoxybenzyl)oxy)phenyl)-4,4-dimethyl-4,5-dihydrooxazole 5d



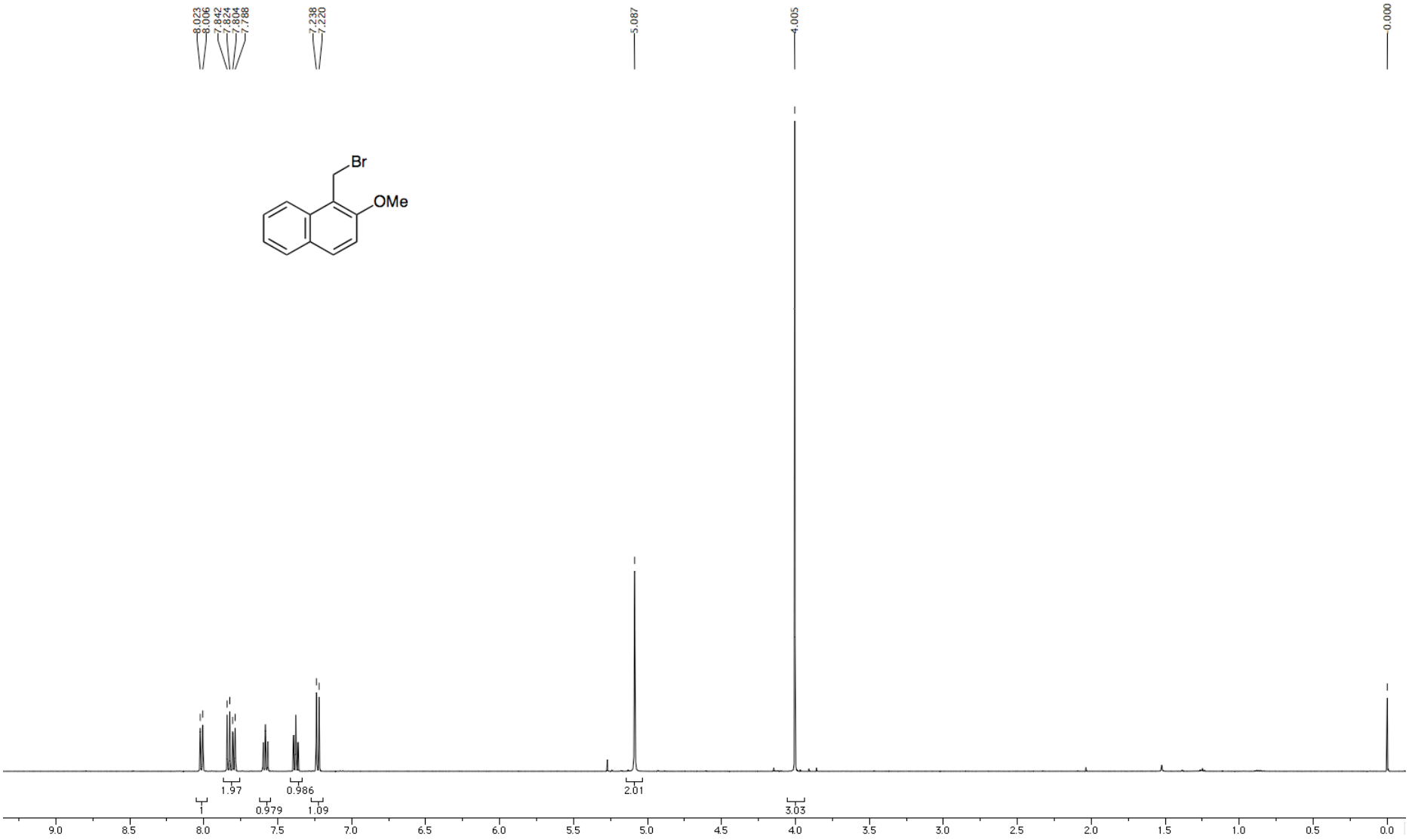
500 MHz ^{1}H NMR Spectrum of (2-Methoxynaphthalen-1-yl)methanol C



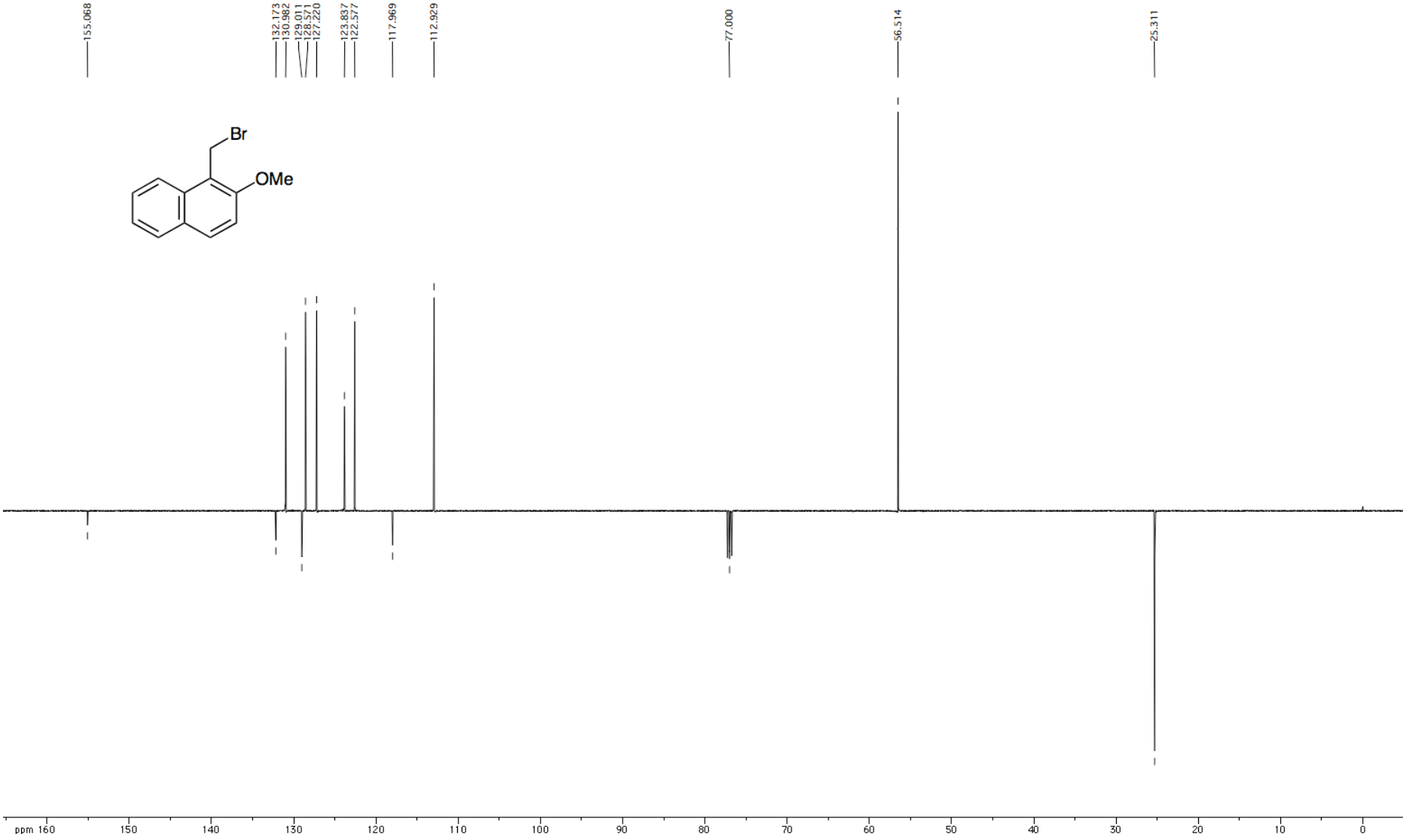
125 MHz DEPTQ ^{13}C NMR Spectrum of (2-Methoxynaphthalen-1-yl)methanol C



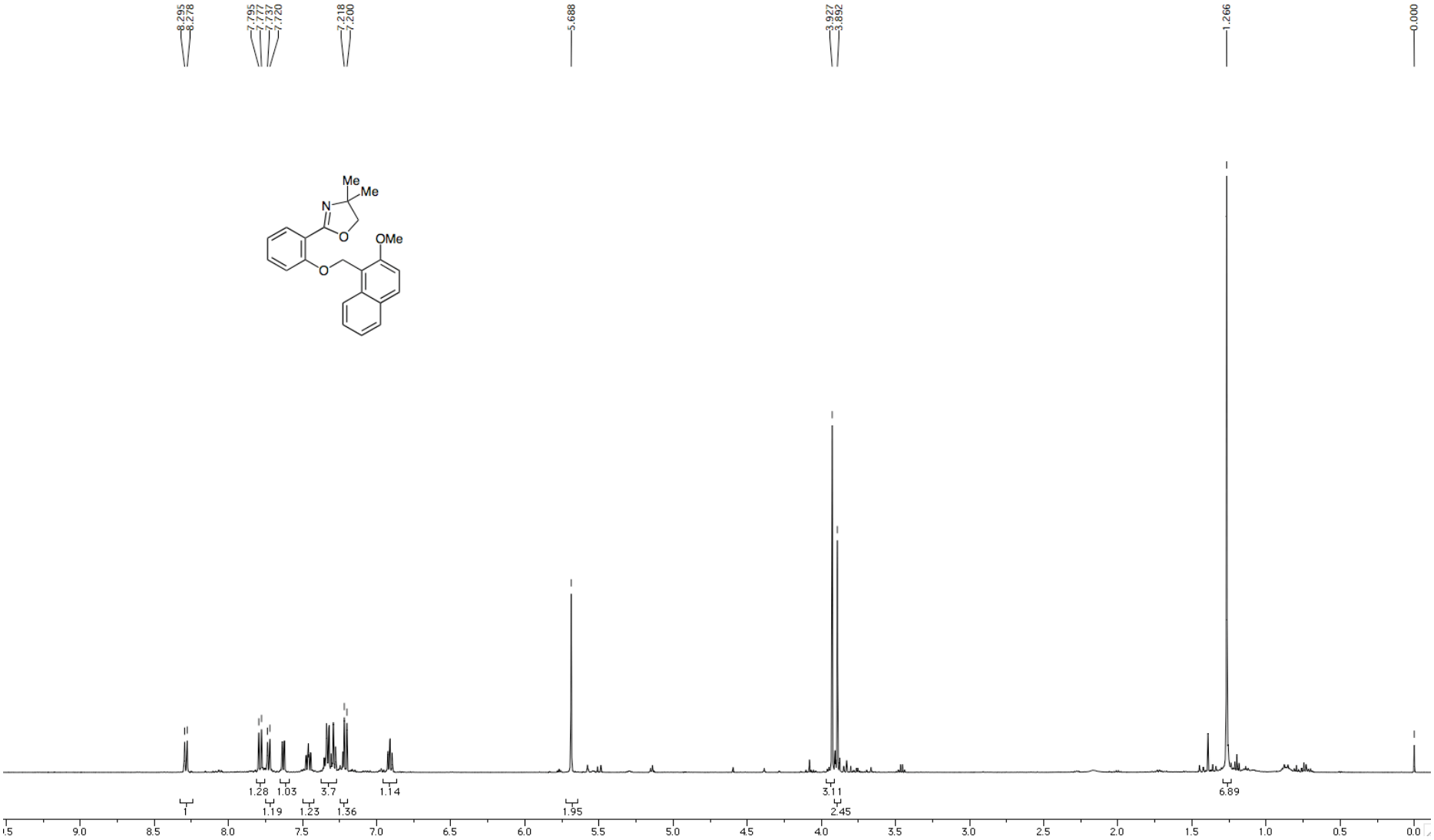
500 MHz ^{1}H NMR Spectrum of 1-(Bromomethyl)-2-methoxynaphthalene D



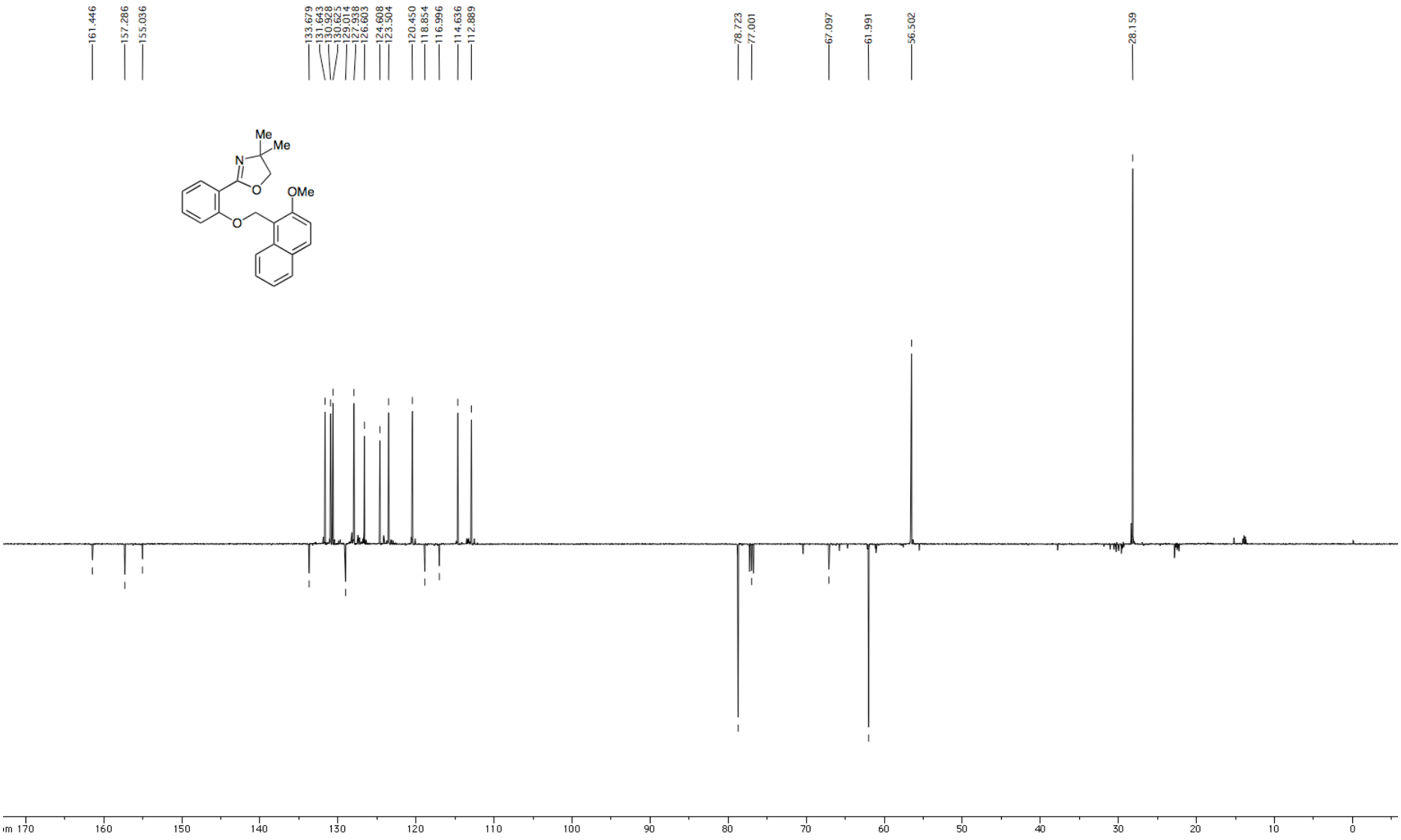
125 MHz DEPTQ ^{13}C NMR Spectrum of 1-(Bromomethyl)-2-methoxynaphthalene D



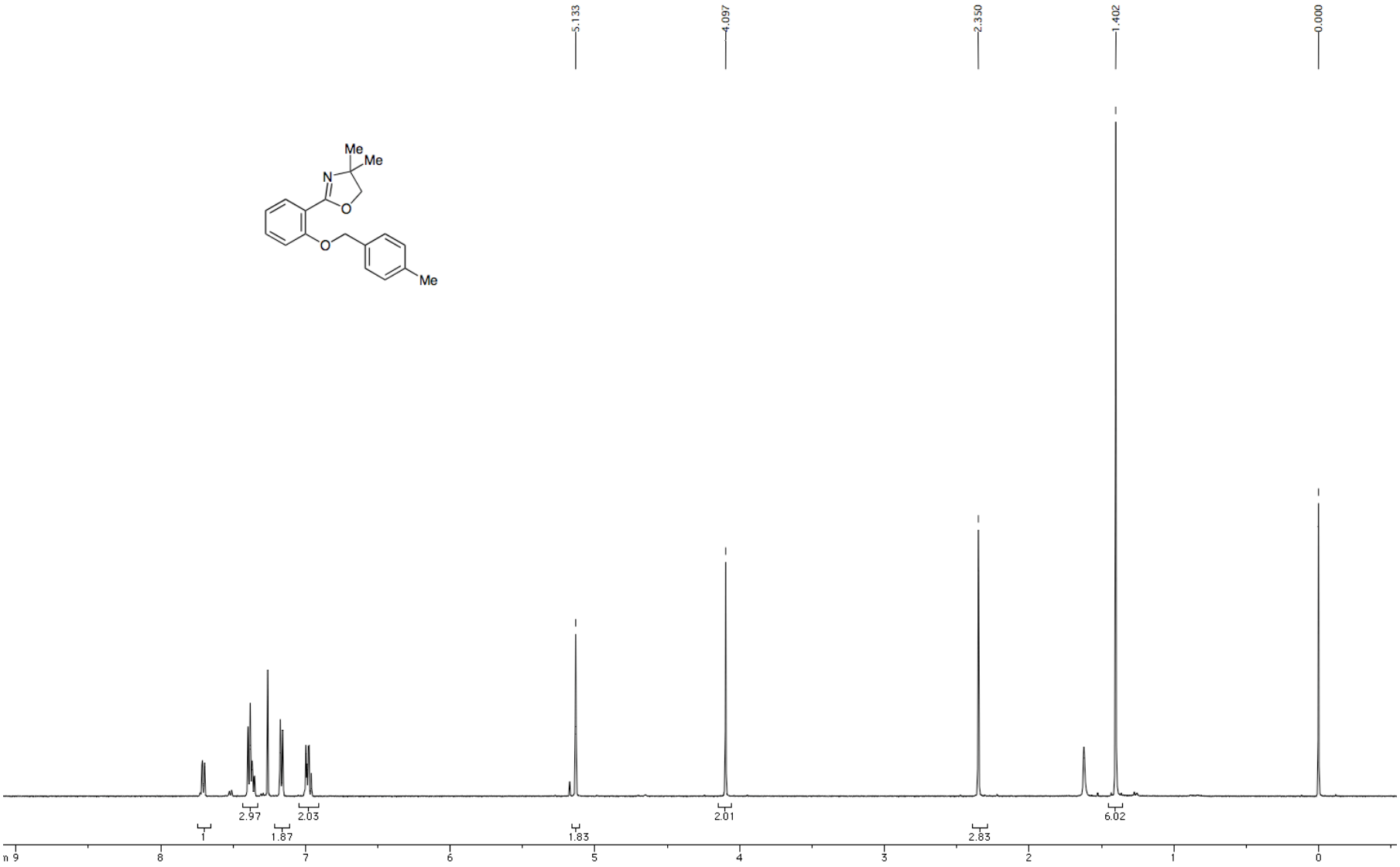
500 MHz ^{1}H NMR Spectrum of 2-(2-((2-Methoxynaphthalen-1-yl)methoxy)phenyl)-4,4-dimethyl-4,5-dihydrooxazole 5e



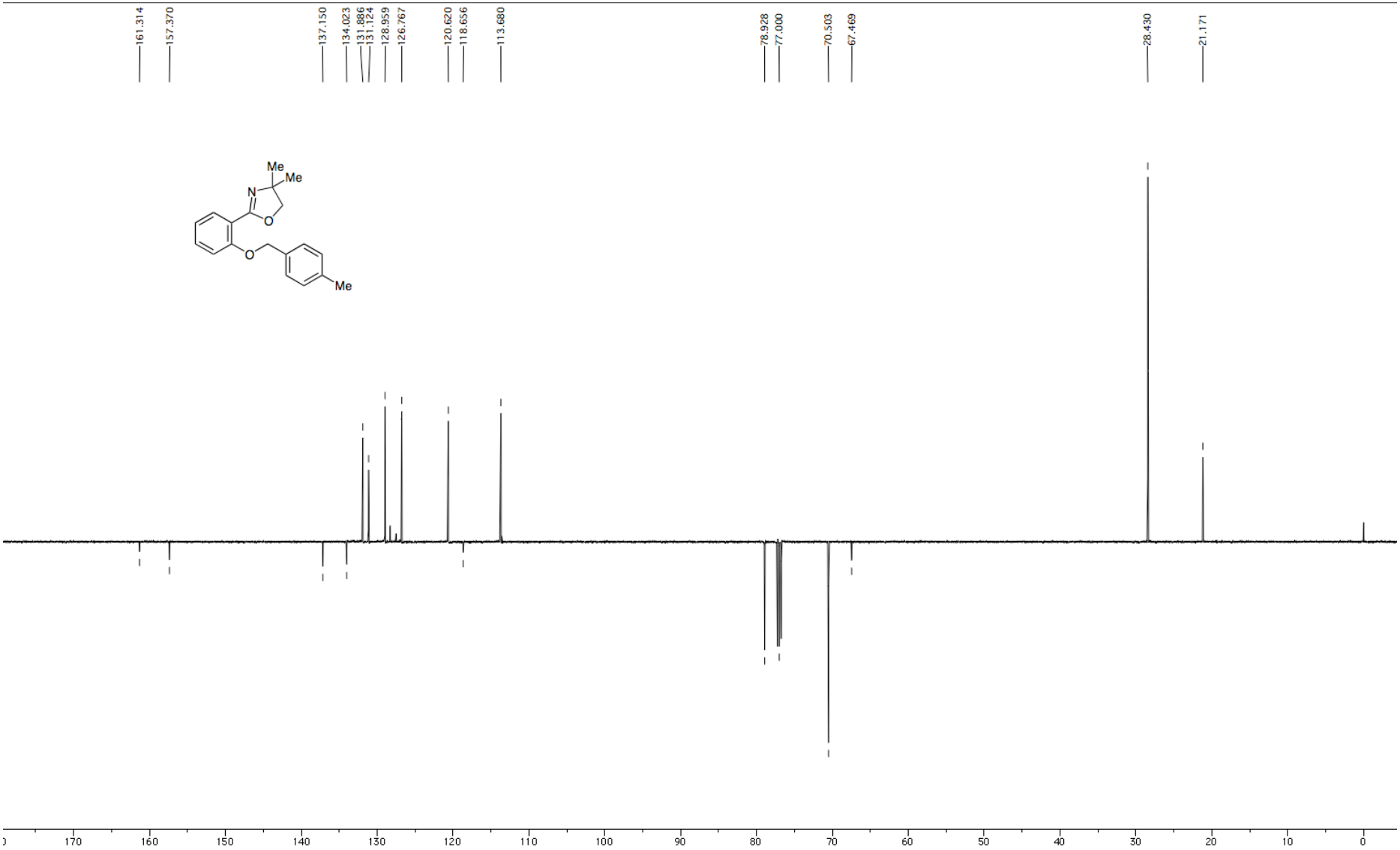
125 MHz DEPTQ ^{13}C NMR Spectrum of 2-(2-((2-Methoxynaphthalen-1-yl)methoxy)phenyl)-4,4-dimethyl-4,5-dihydrooxazole 5e



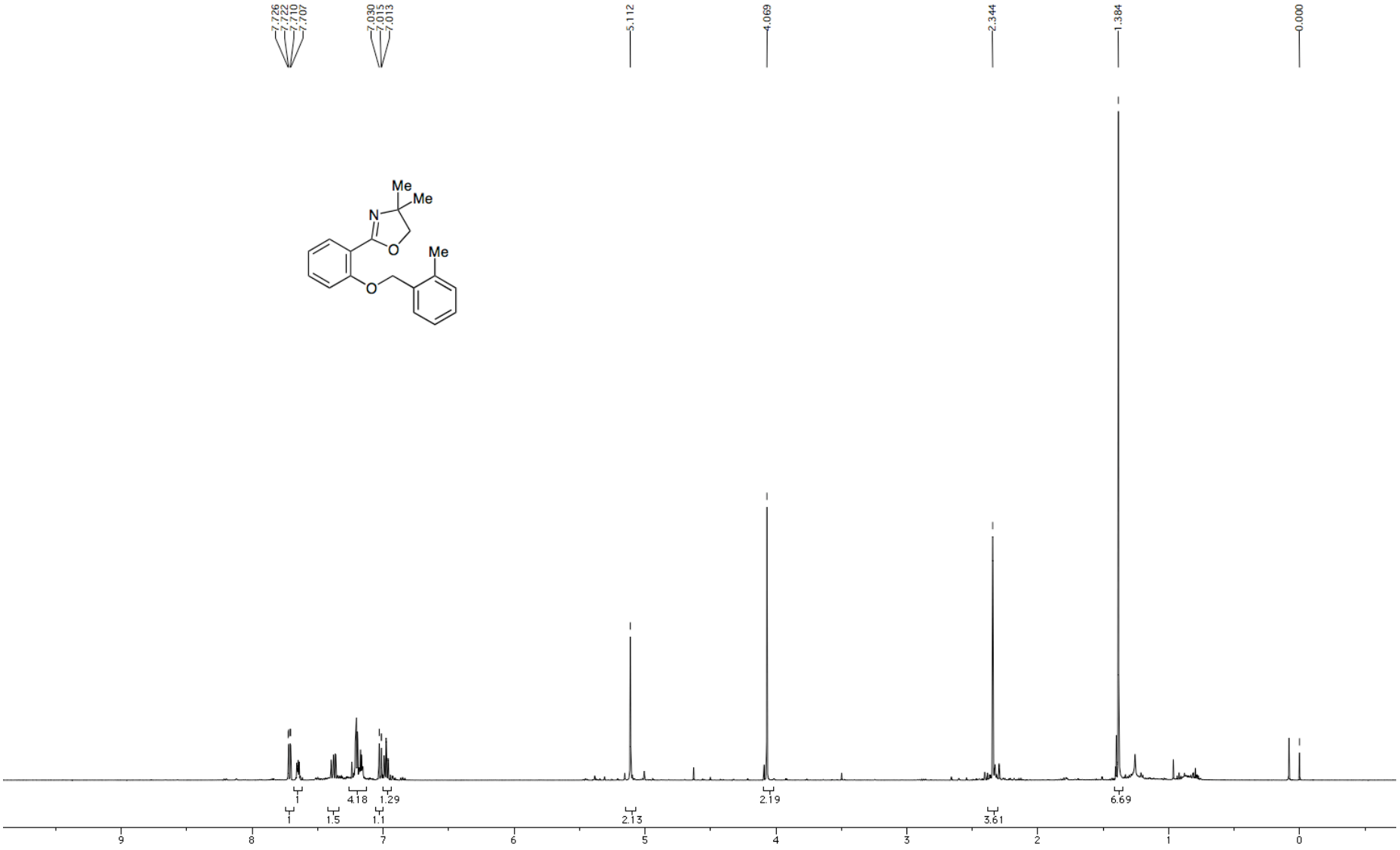
500 MHz ^{1}H NMR Spectrum of 4,4-Dimethyl-2-(2-((4-methylbenzyl)oxy)phenyl)-4,5-dihydrooxazole 5f



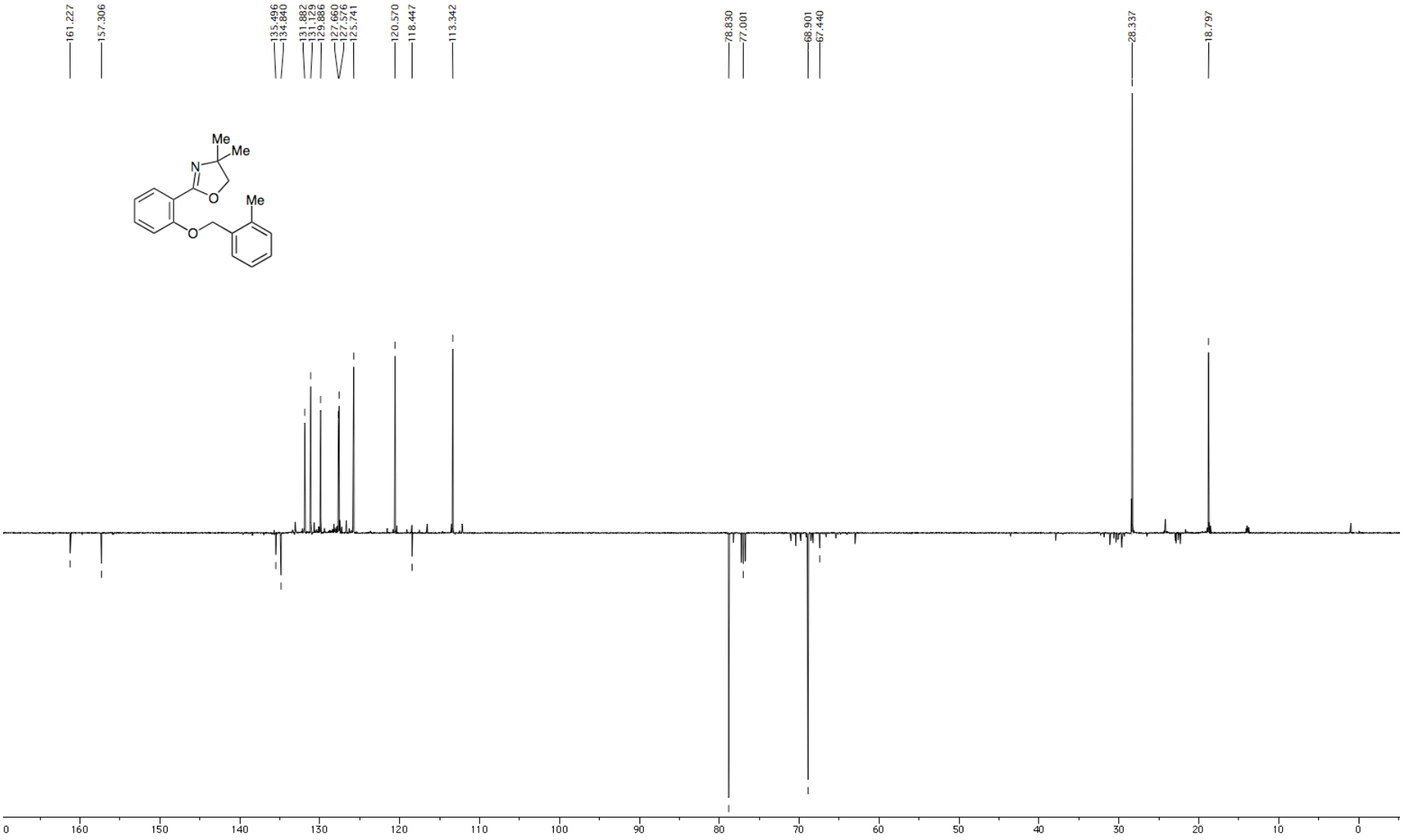
125 MHz DEPTQ ^{13}C NMR Spectrum of 4,4-Dimethyl-2-(2-((4-methylbenzyl)oxy)phenyl)-4,5-dihydrooxazole 5f



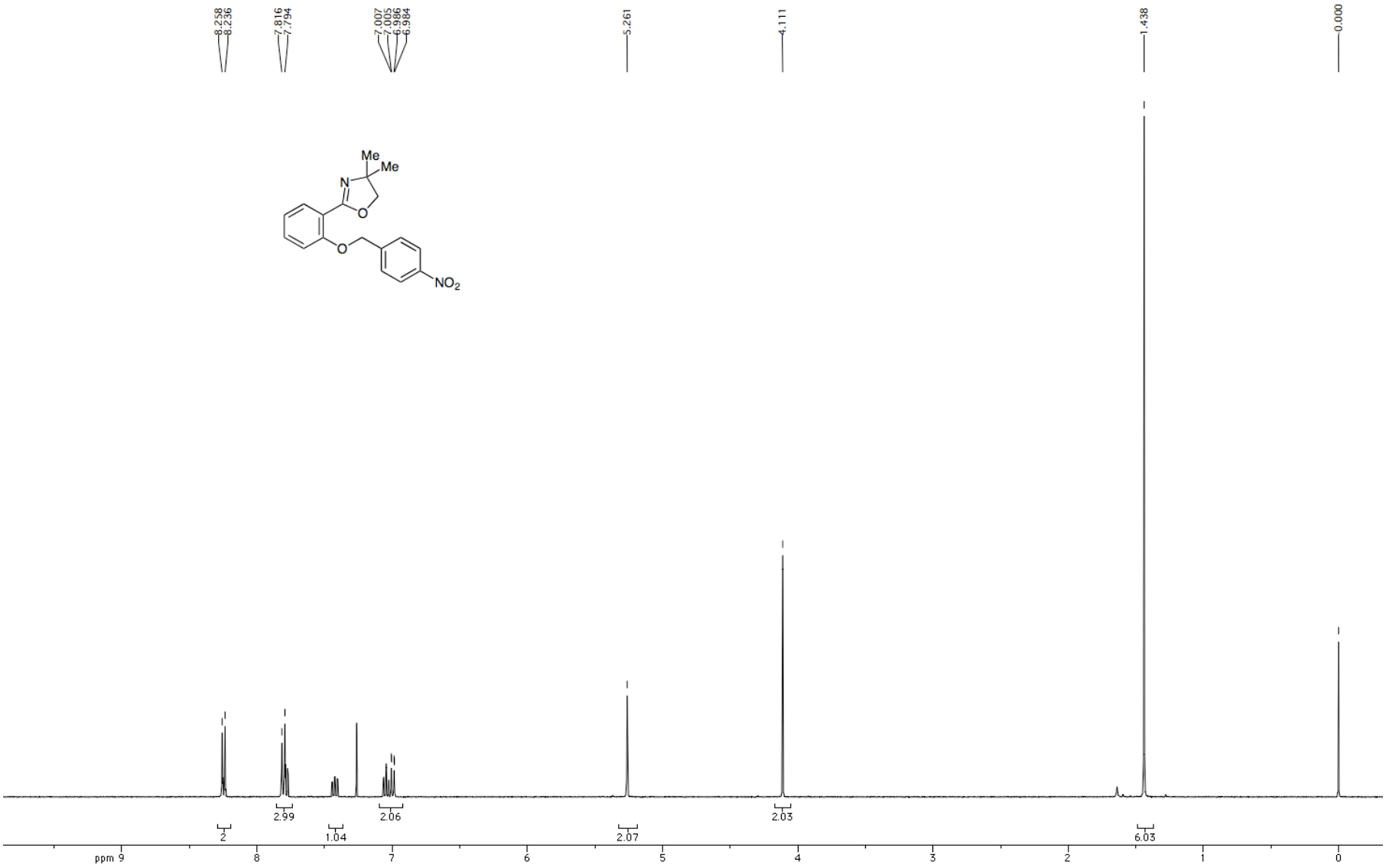
500 MHz ^{1}H NMR Spectrum of 4,4-Dimethyl-2-(2-((2-methylbenzyl)oxy)phenyl)-4,5-dihydrooxazole 5g



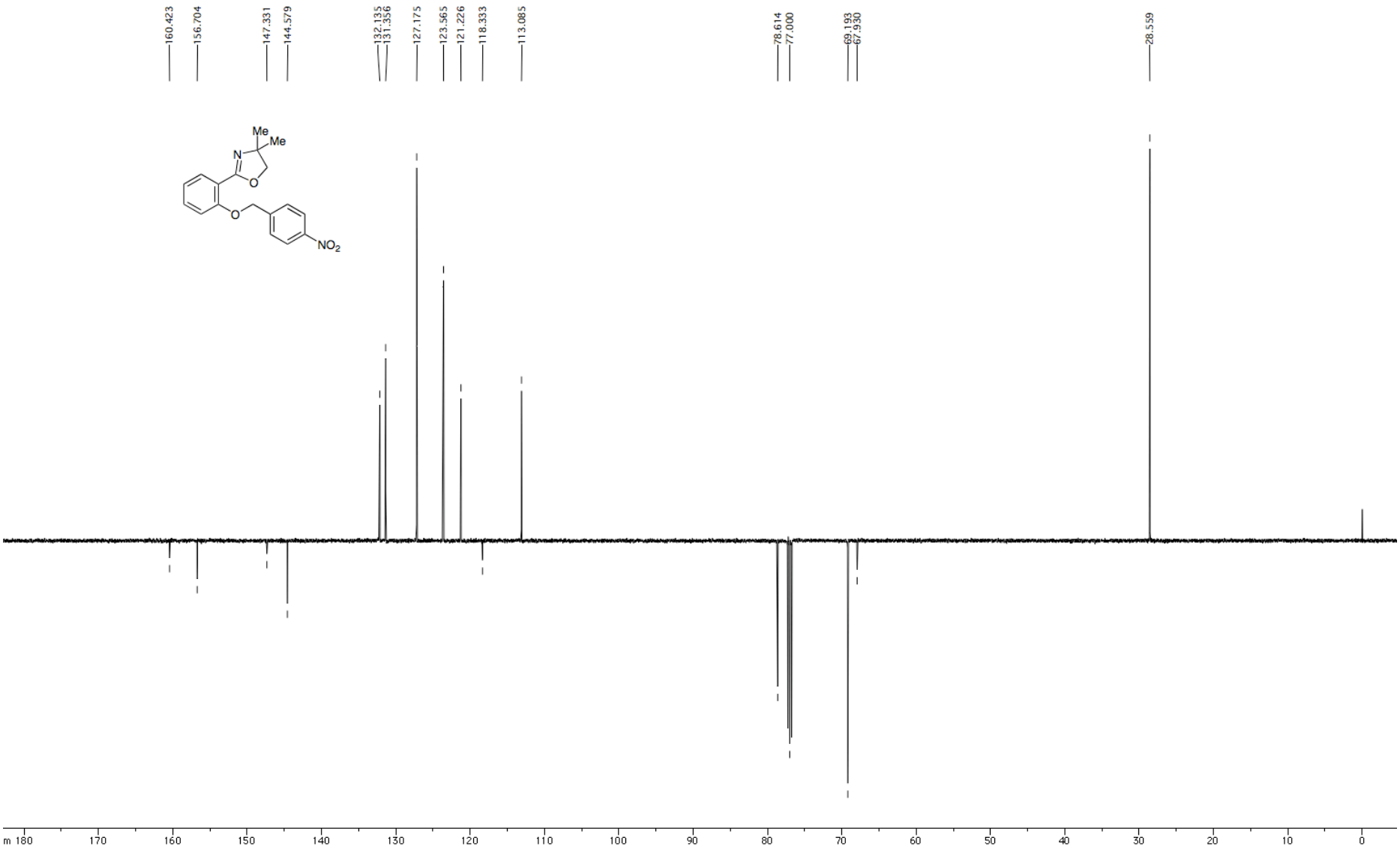
125 MHz DEPTQ ^{13}C NMR Spectrum of 4,4-Dimethyl-2-(2-((2-methylbenzyl)oxy)phenyl)-4,5-dihydrooxazole 5g



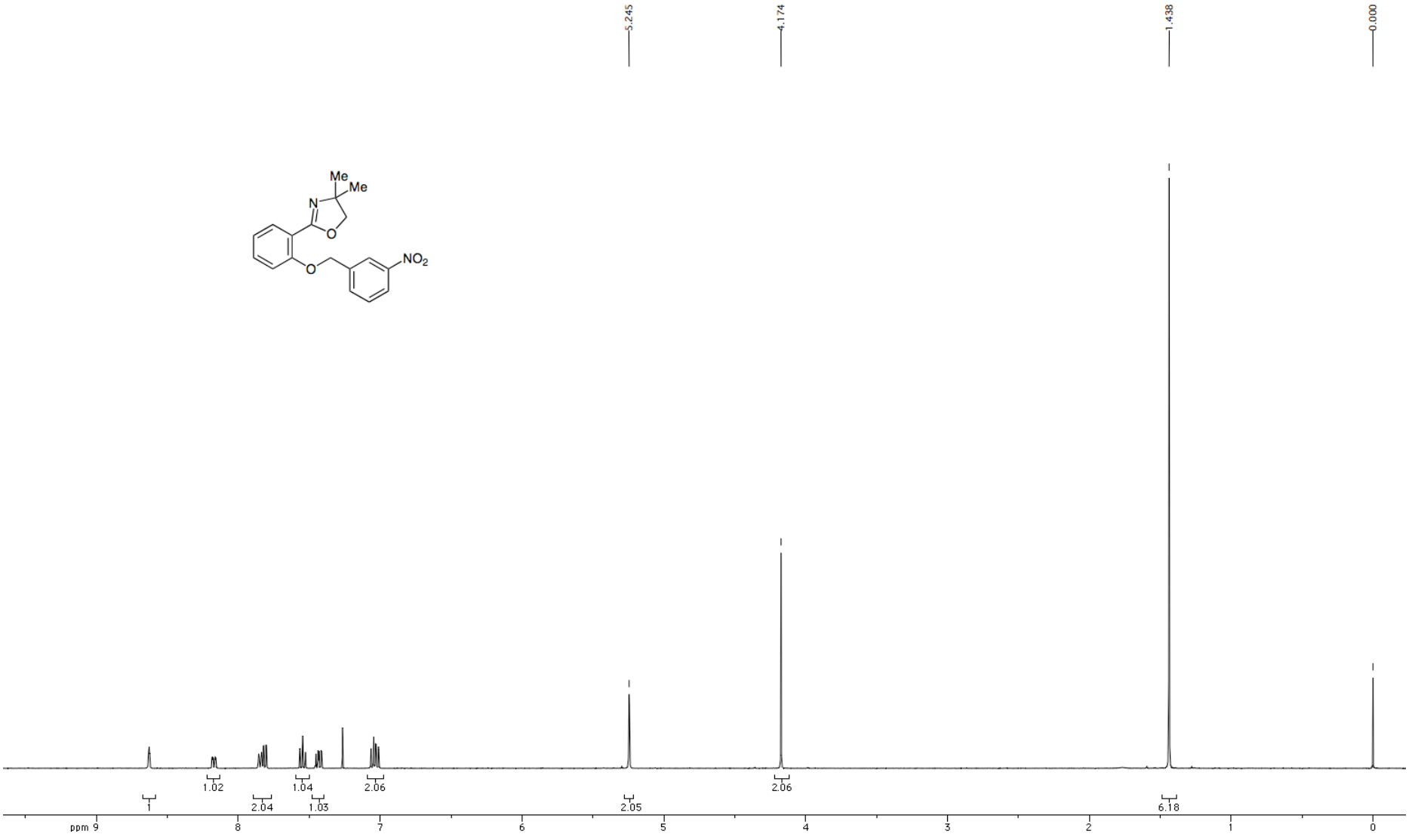
400 MHz ^{1}H NMR Spectrum of 4,4-Dimethyl-2-(2-((4-nitrobenzyl)oxy)phenyl)-4,5-dihydrooxazole 5h



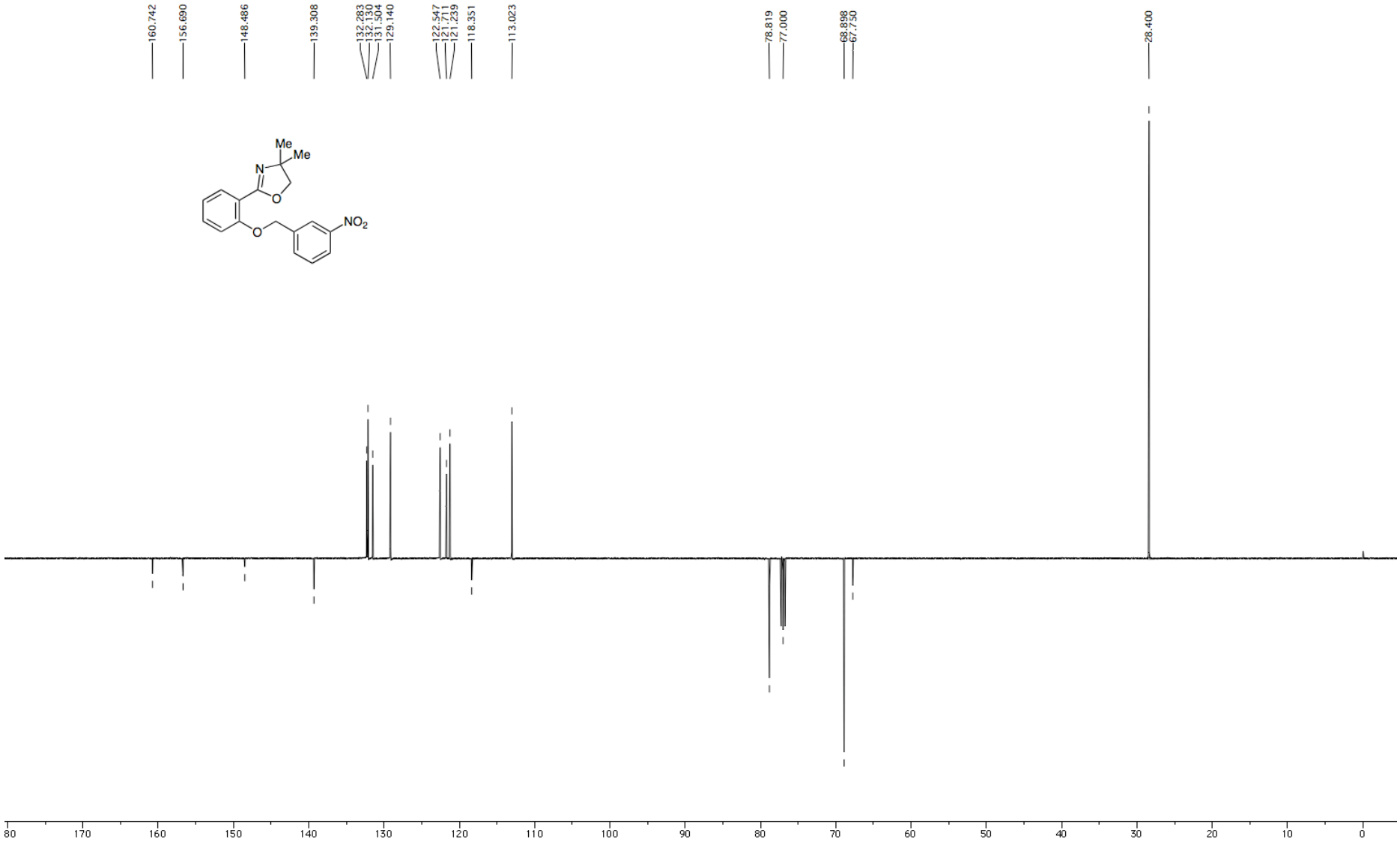
125 MHz DEPTQ ^{13}C NMR Spectrum of 4,4-Dimethyl-2-(2-((4-nitrobenzyl)oxy)phenyl)-4,5-dihydrooxazole 5h



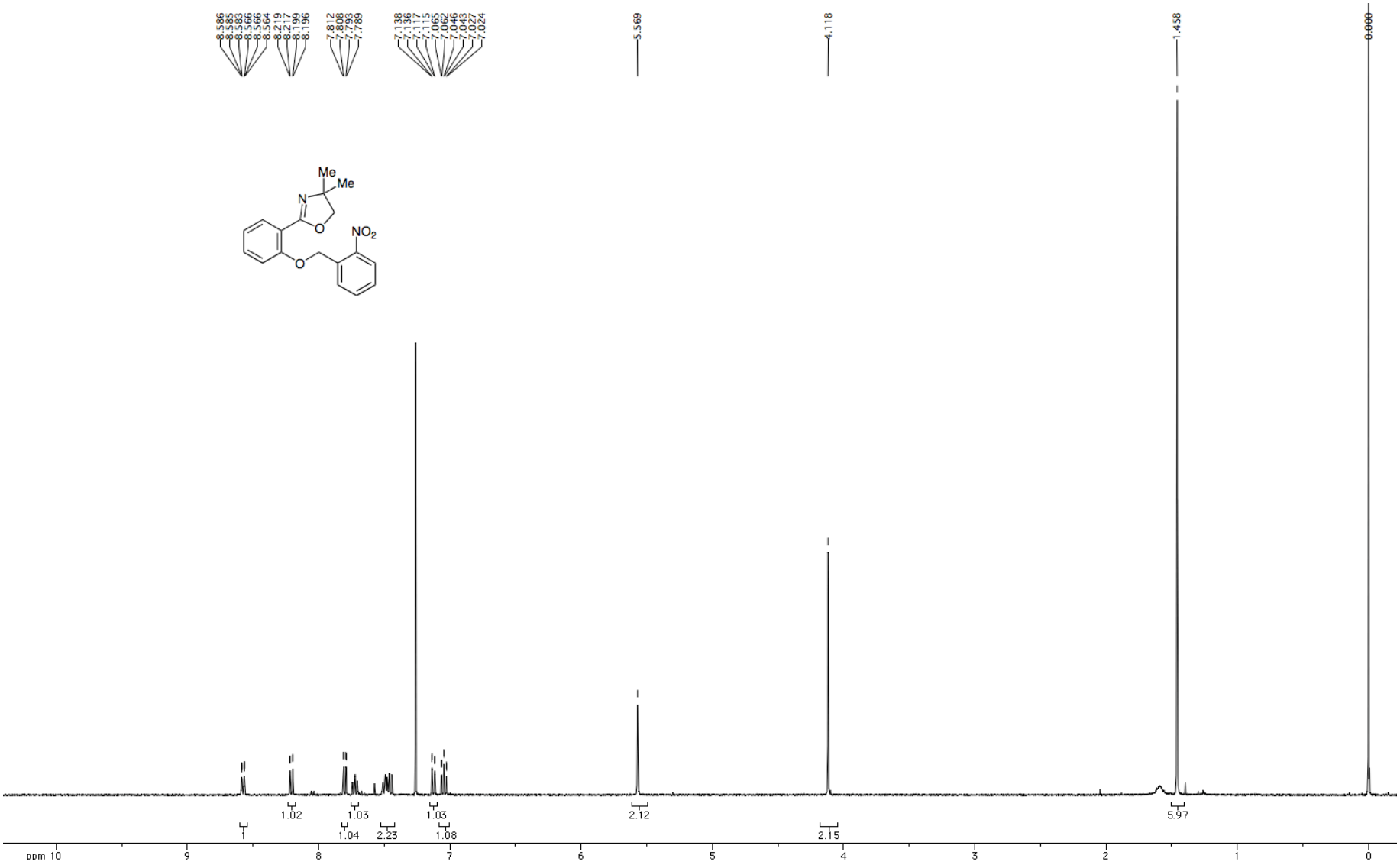
400 MHz ^{1}H NMR Spectrum of 4,4-Dimethyl-2-(2-((3-nitrobenzyl)oxy)phenyl)-4,5-dihydrooxazole 5i



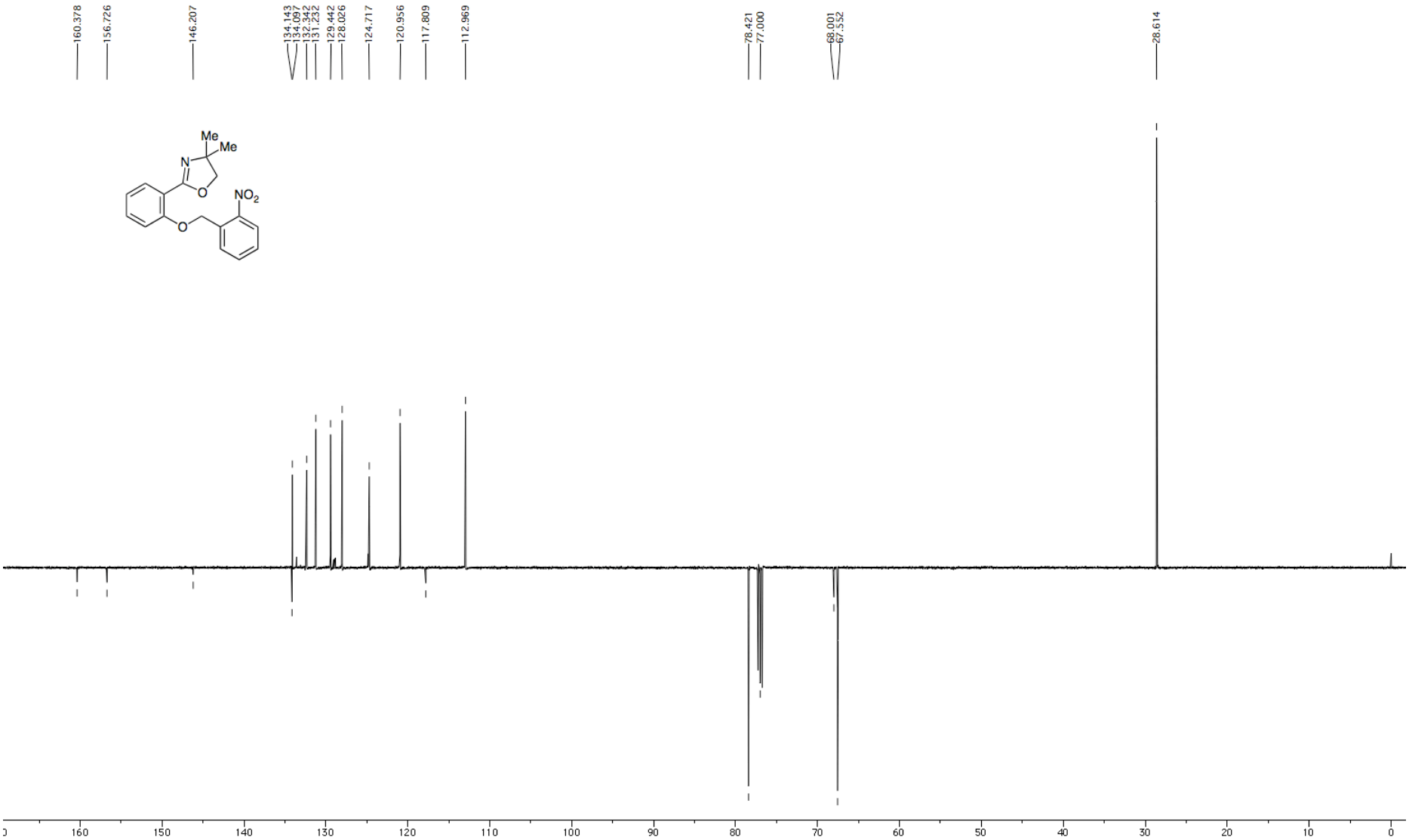
125 MHz DEPTQ ^{13}C NMR Spectrum of 4,4-Dimethyl-2-(2-((3-nitrobenzyl)oxy)phenyl)-4,5-dihydrooxazole 5i



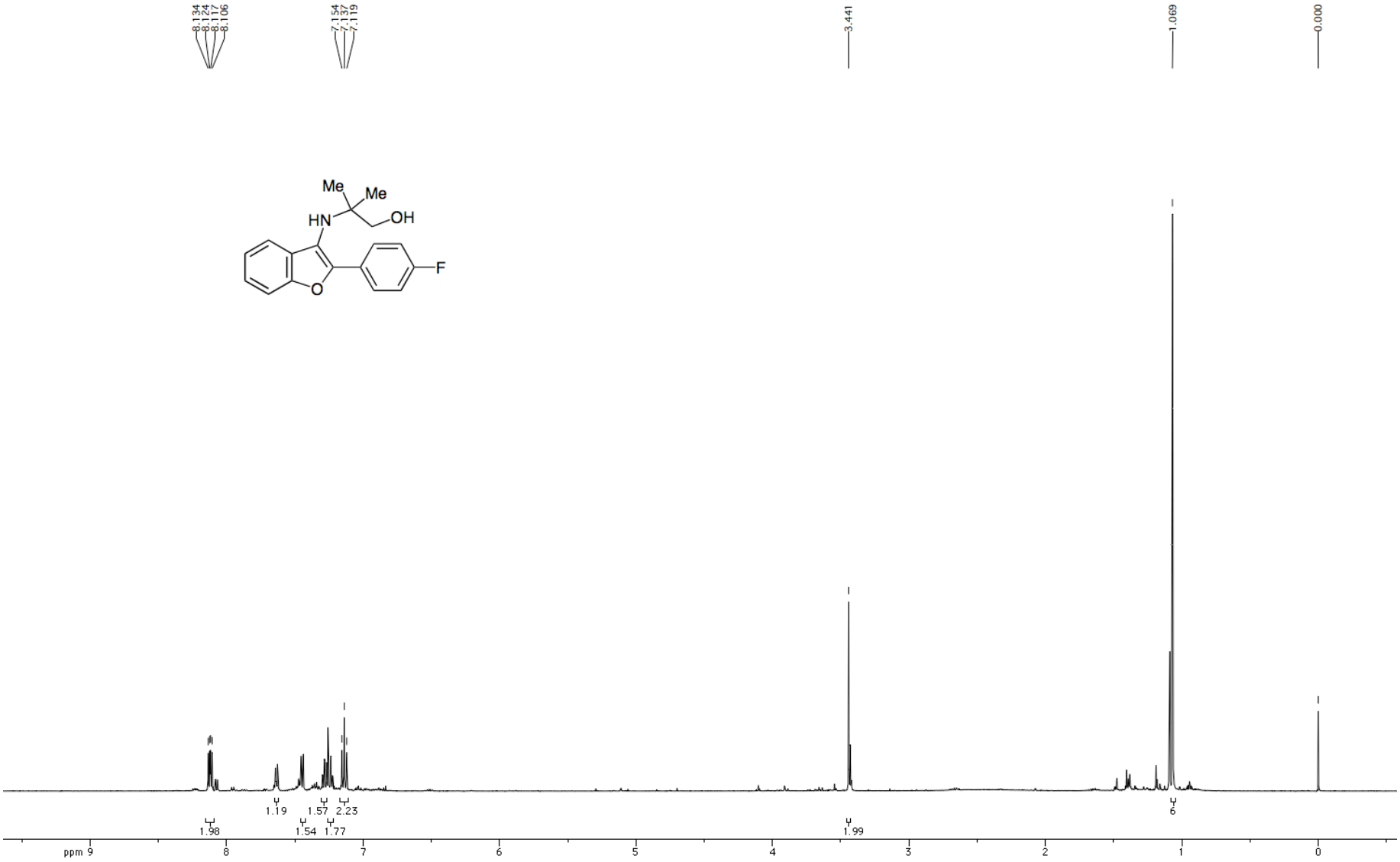
400 MHz ^{1}H NMR Spectrum of 4,4-Dimethyl-2-(2-((2-nitrobenzyl)oxy)phenyl)-4,5-dihydrooxazole 5j



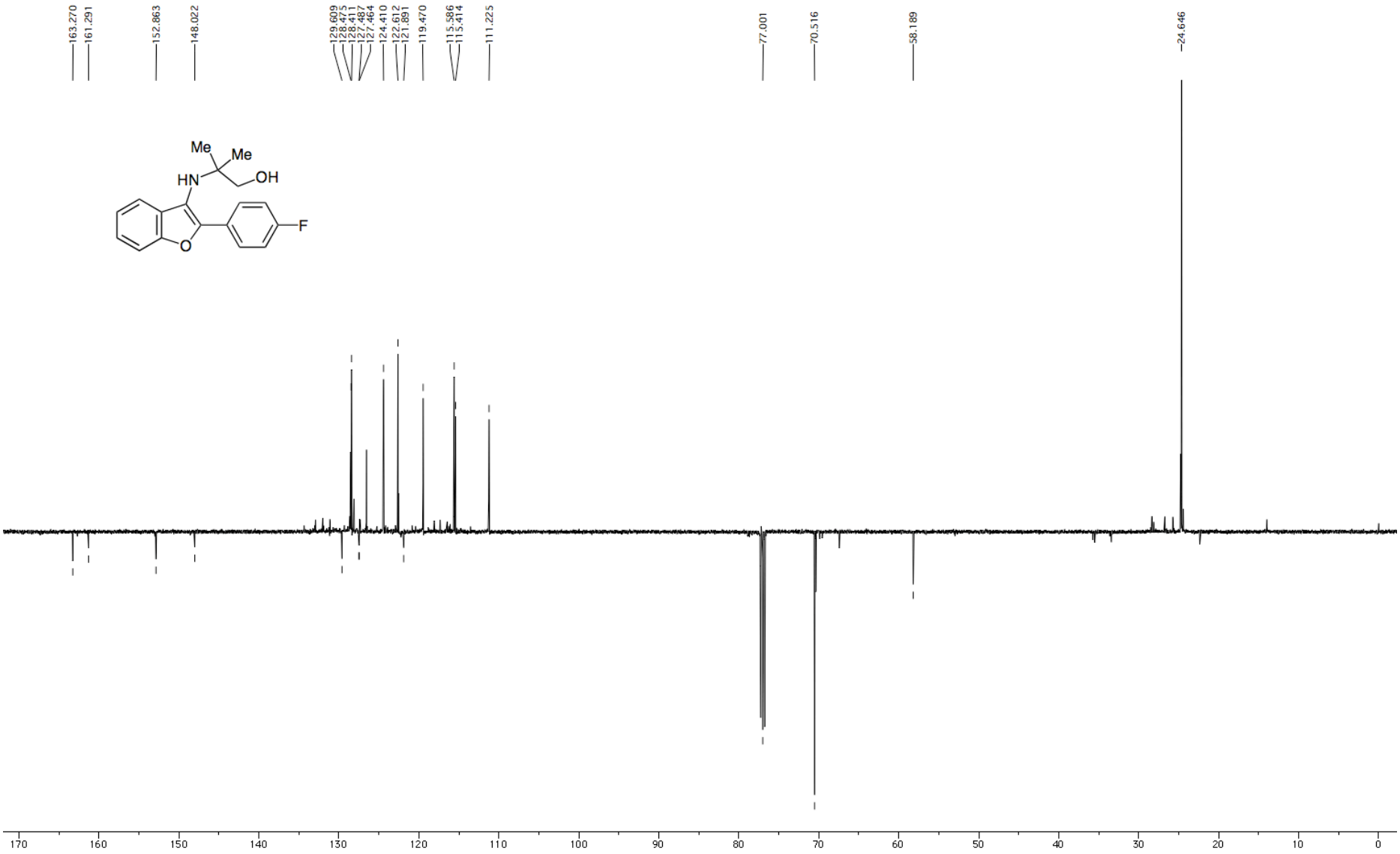
125 MHz DEPTQ ^{13}C NMR Spectrum of 4,4-Dimethyl-2-(2-((2-nitrobenzyl)oxy)phenyl)-4,5-dihydrooxazole 5j



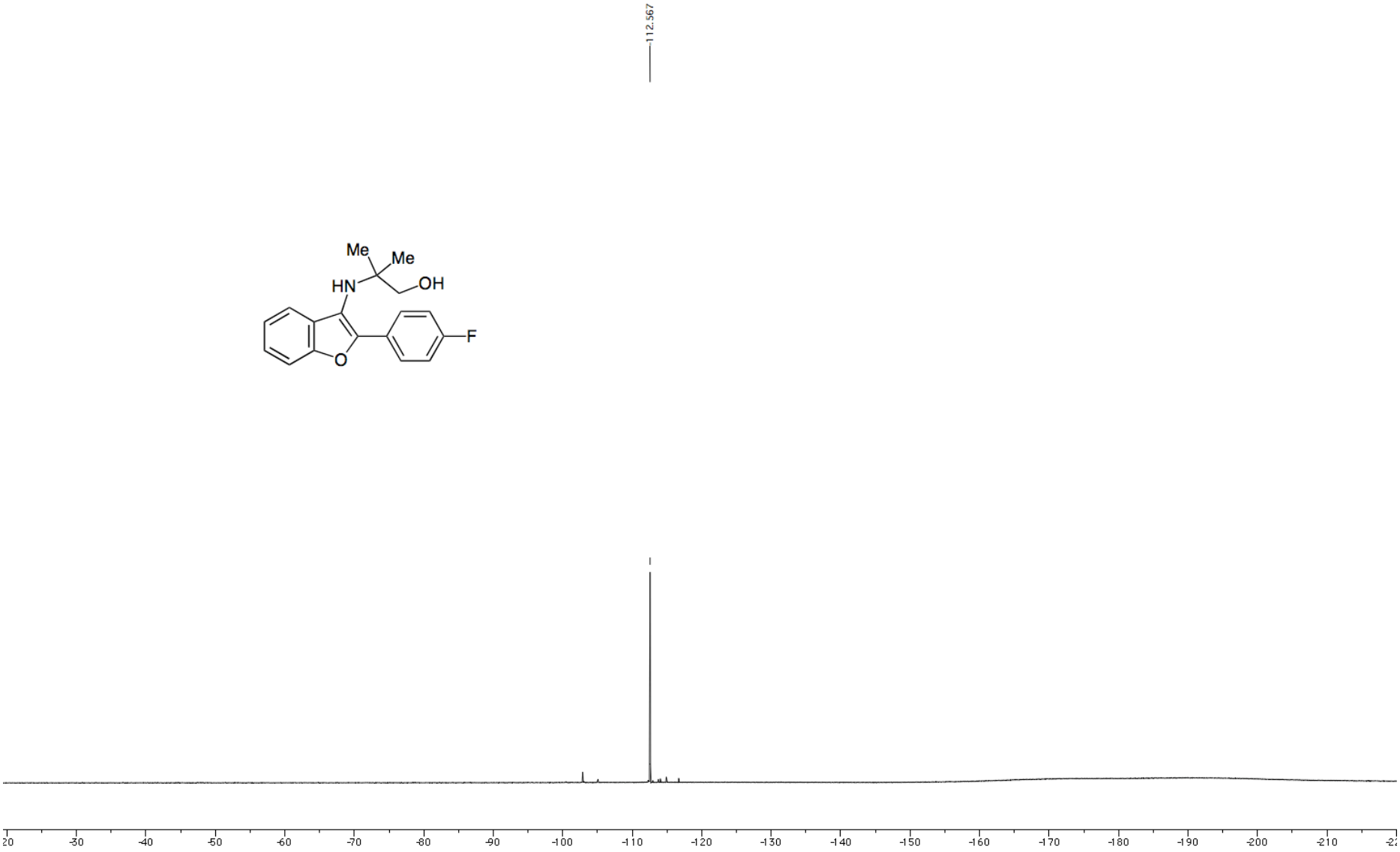
500 MHz ^{1}H NMR Spectrum of 2-((2-(4-Fluorophenyl)benzofuran-3-yl)amino)-2-methylpropan-1-ol 6a



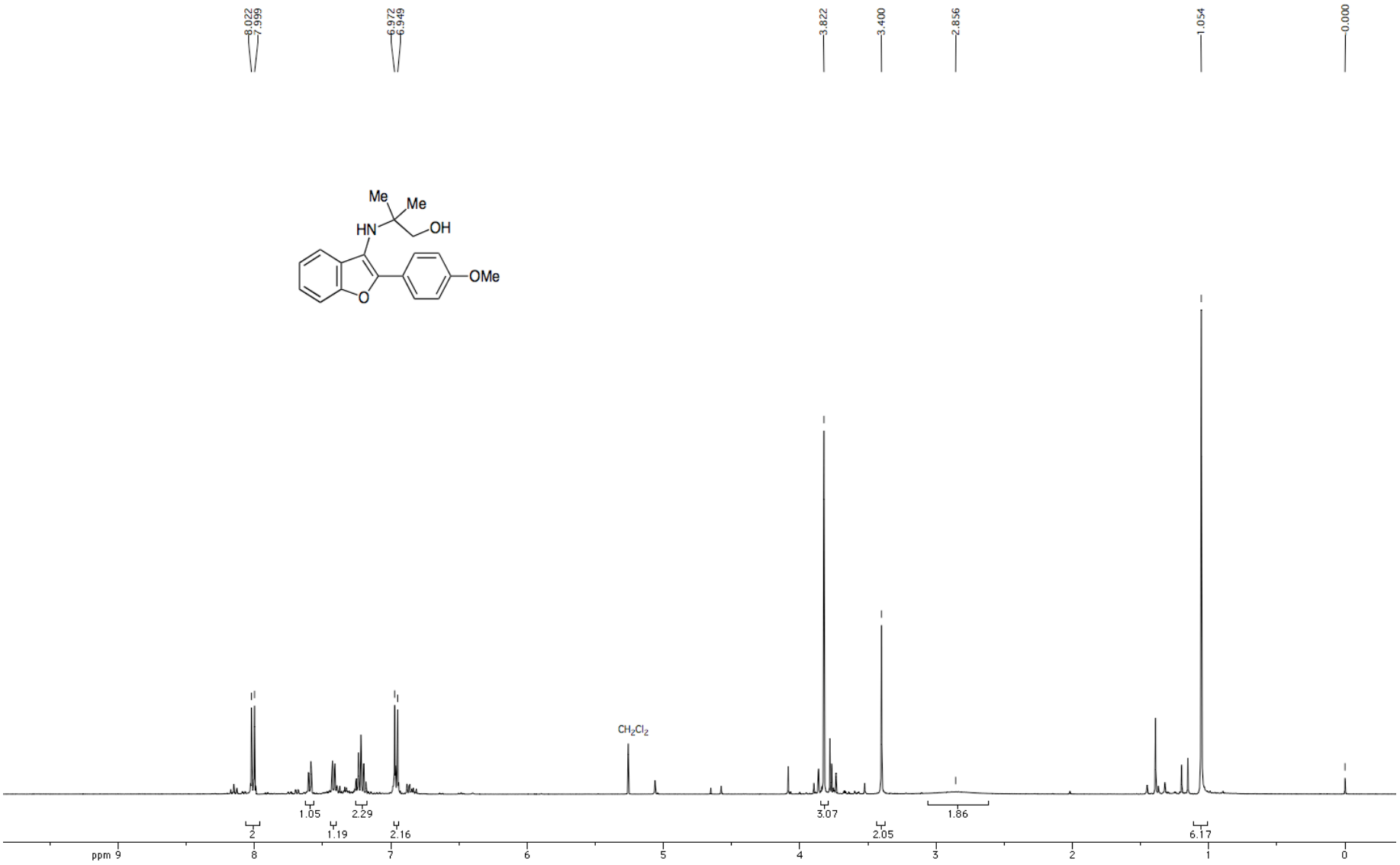
125 MHz DEPTQ ^{13}C NMR Spectrum of 2-((2-(4-Fluorophenyl)benzofuran-3-yl)amino)-2-methylpropan-1-ol 6a



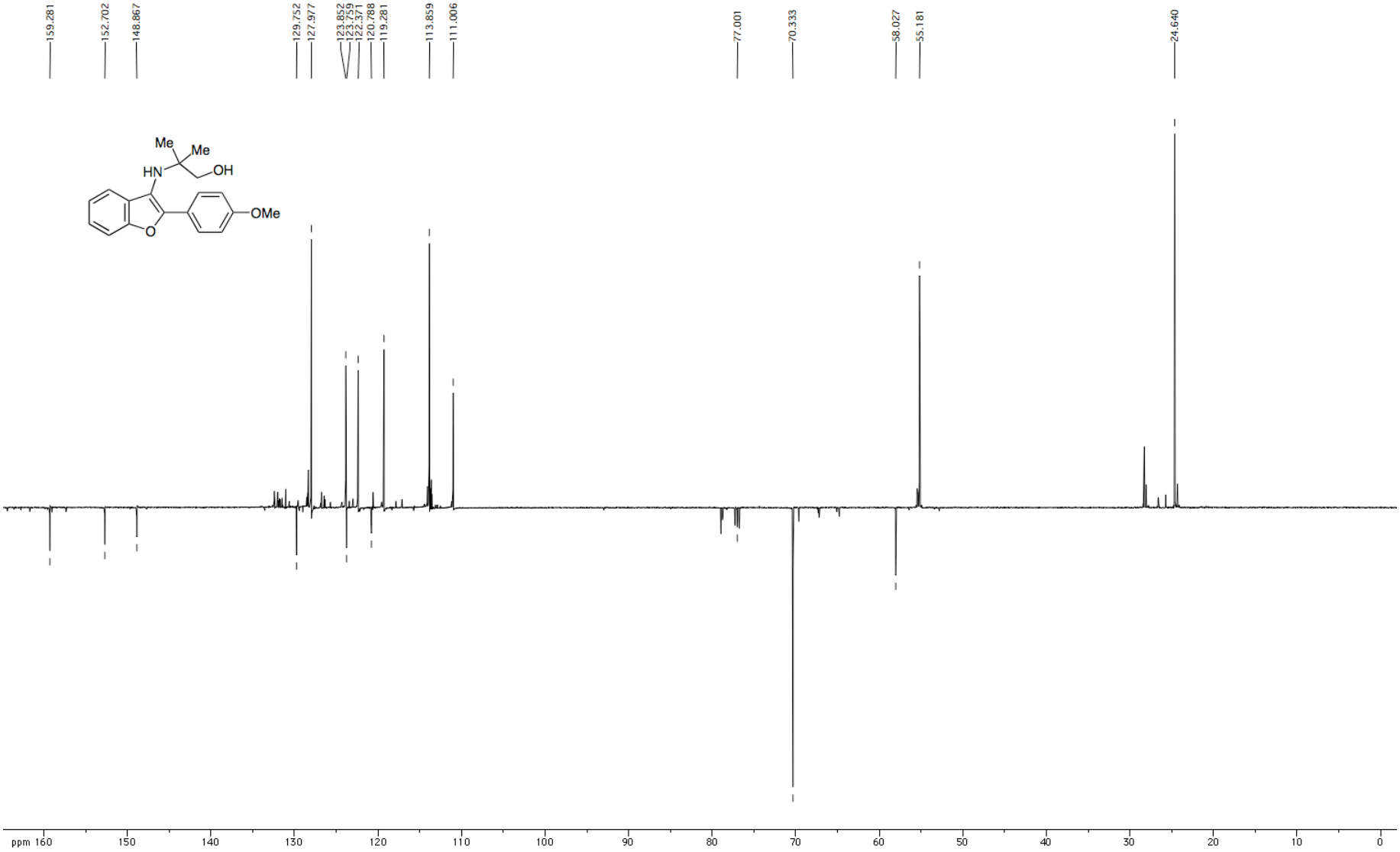
376 MHz ^{19}F NMR Spectrum of 2-((2-(4-Fluorophenyl)benzofuran-3-yl)amino)-2-methylpropan-1-ol 6a



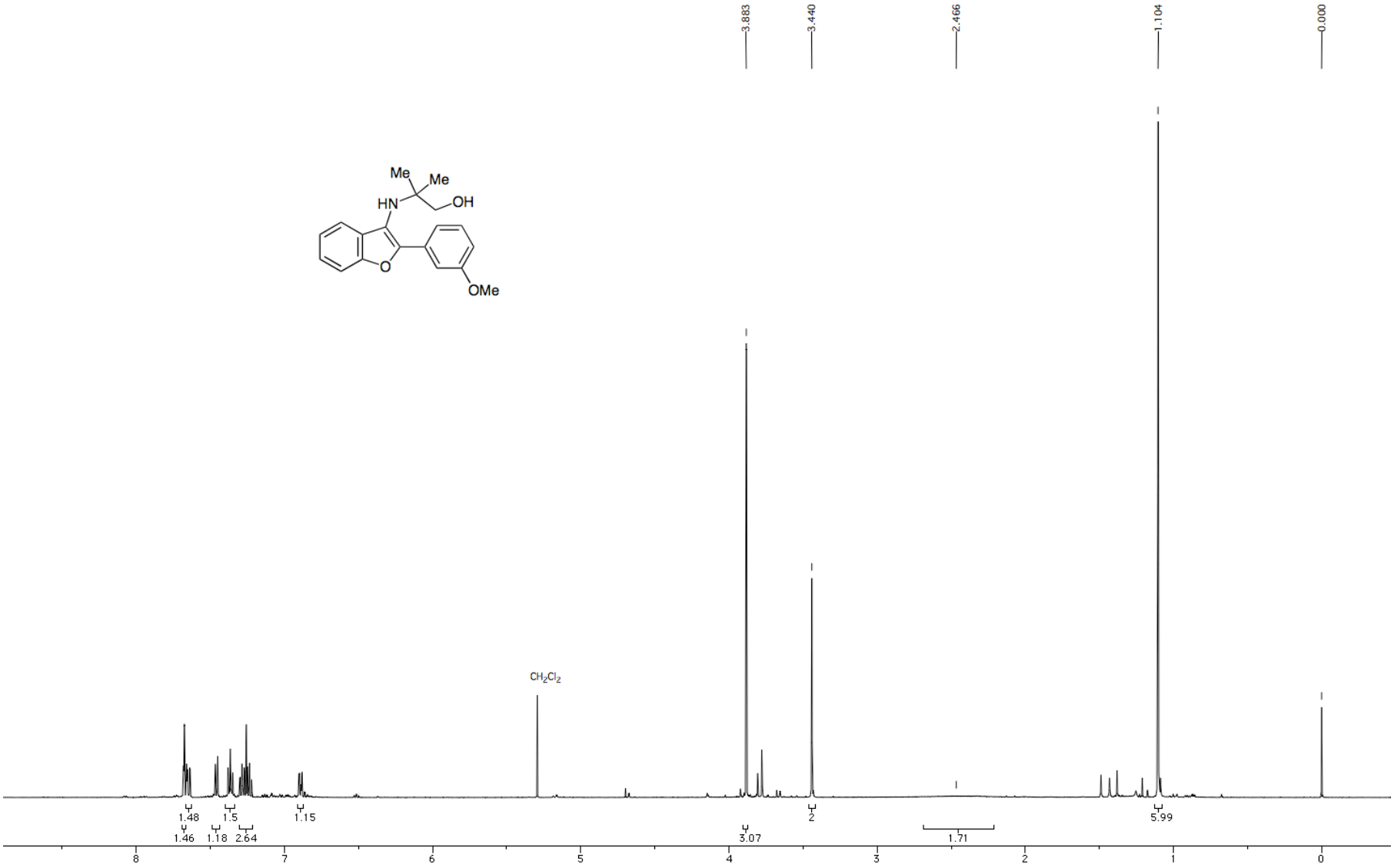
400 MHz ^{1}H NMR Spectrum of 2-((2-(4-Methoxyphenyl)benzofuran-3-yl)amino)-2-methylpropan-1-ol 6b



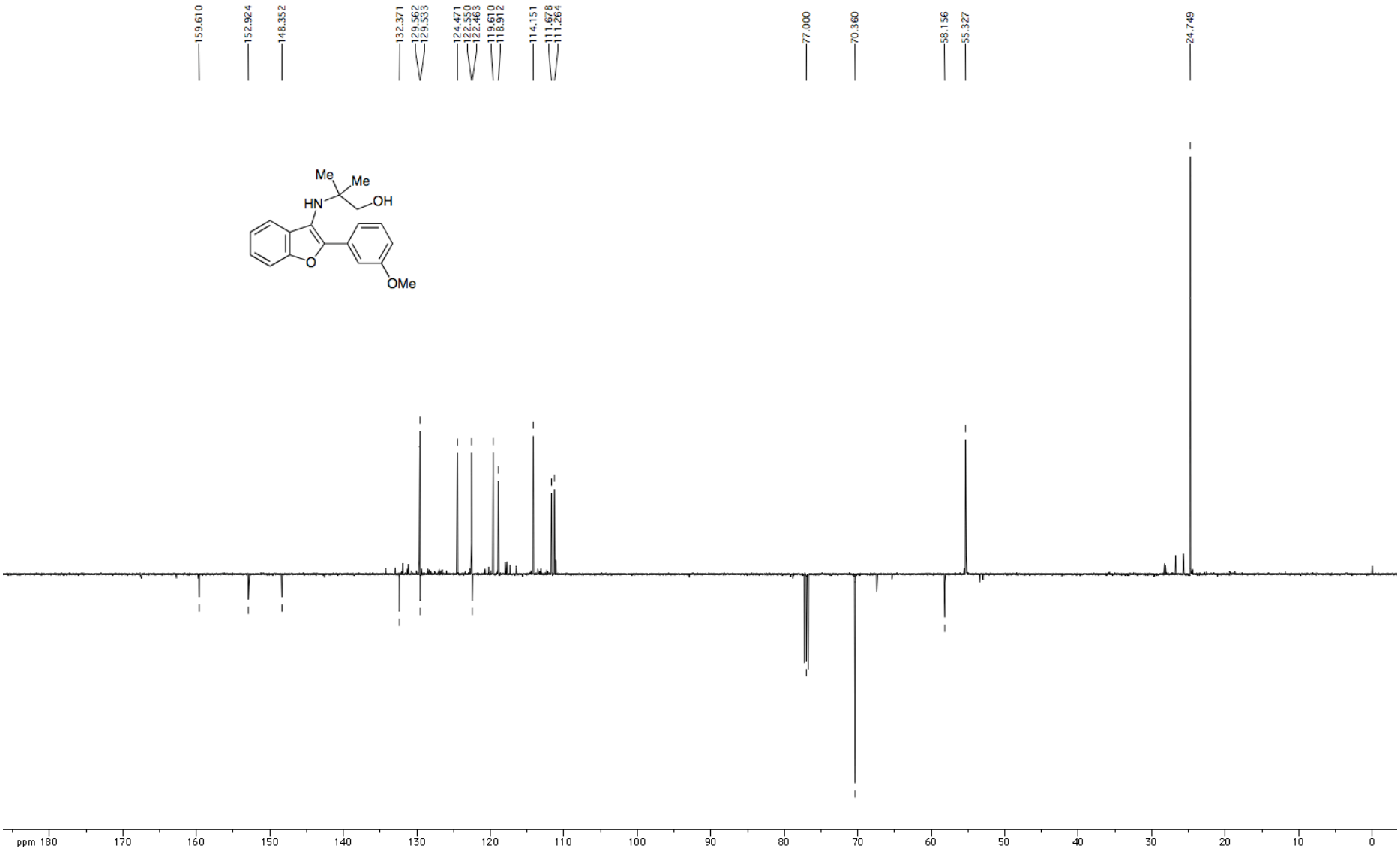
125 MHz DEPTQ ^{13}C NMR Spectrum of 2-((2-(4-Methoxyphenyl)benzofuran-3-yl)amino)-2-methylpropan-1-ol 6b



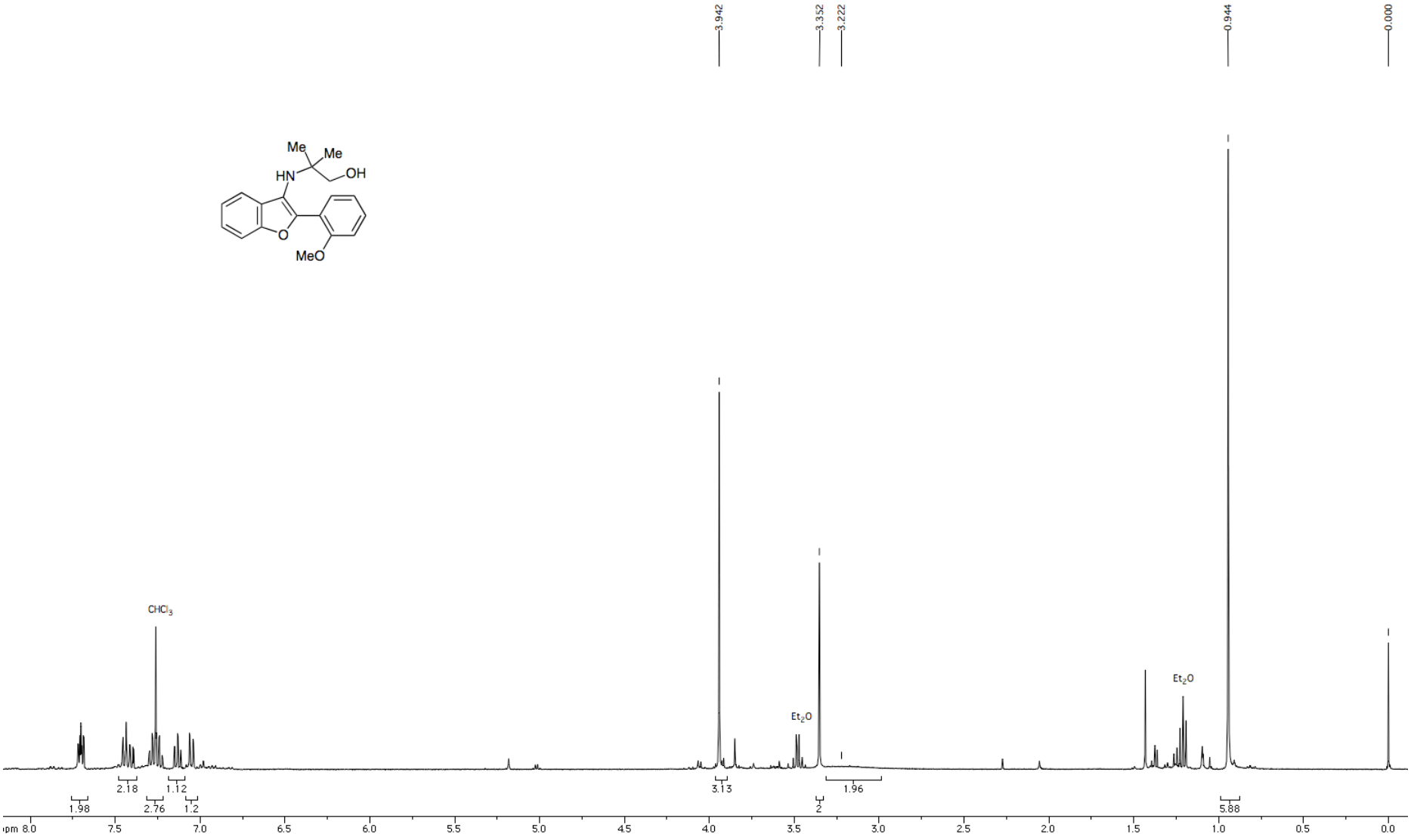
500 MHz ^{1}H NMR Spectrum of 2-((2-(3-Methoxyphenyl)benzofuran-3-yl)amino)-2-methylpropan-1-ol 6c



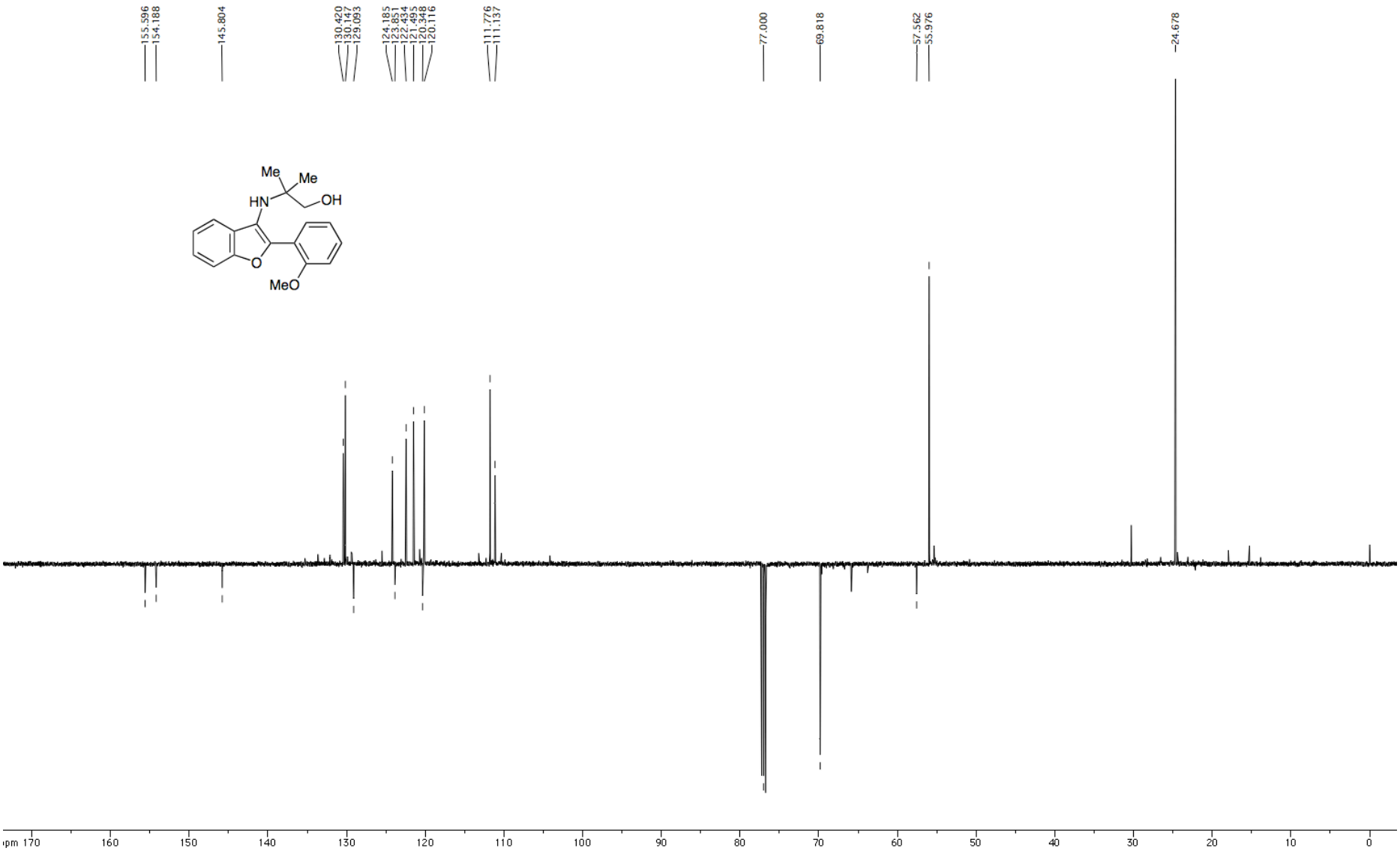
125 MHz DEPTQ ^{13}C NMR Spectrum of 2-((2-(3-Methoxyphenyl)benzofuran-3-yl)amino)-2-methylpropan-1-ol 6c



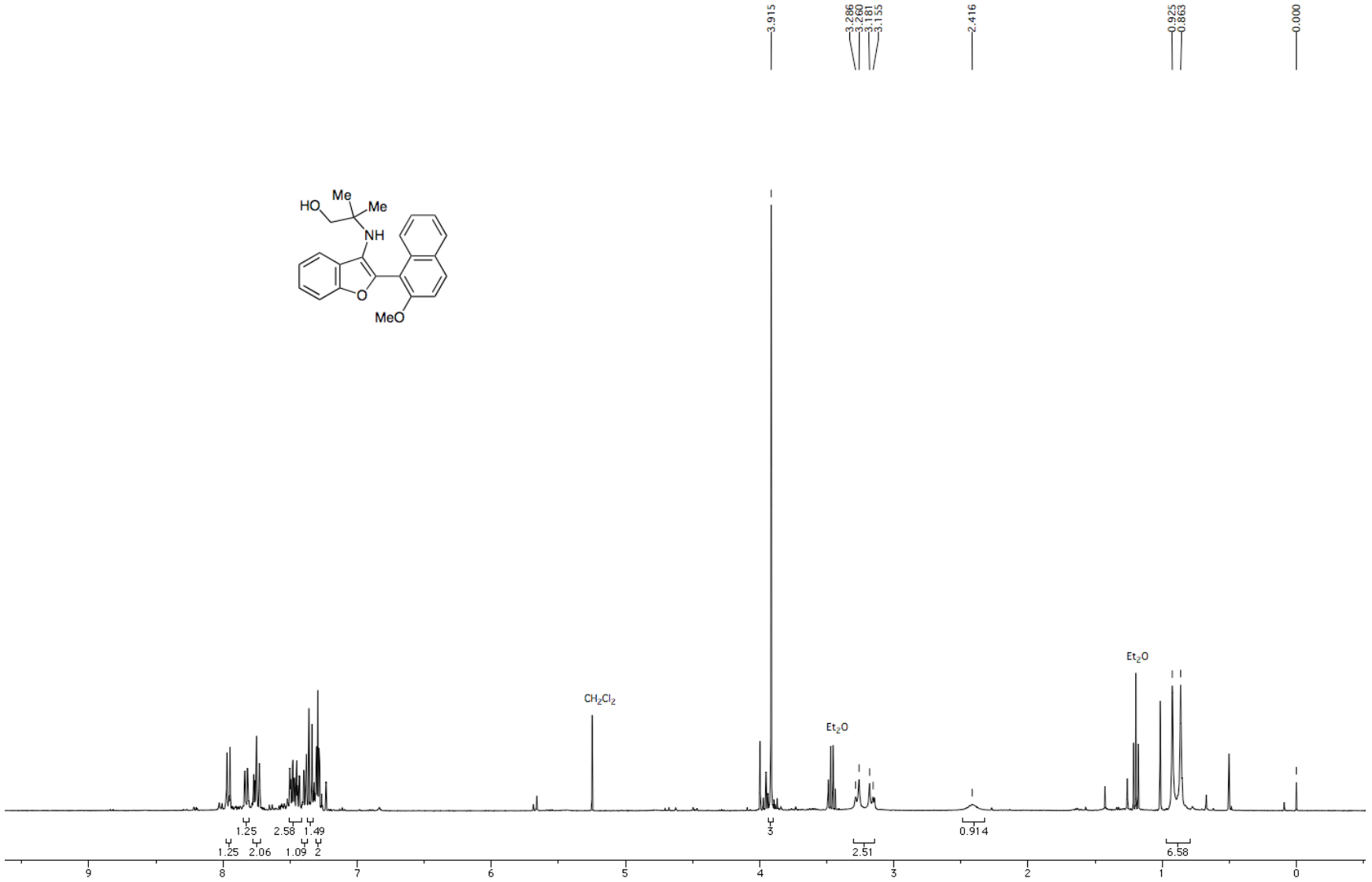
400 MHz ^{1}H NMR Spectrum of 2-((2-(2-Methoxyphenyl)benzofuran-3-yl)amino)-2-methylpropan-1-ol 6d



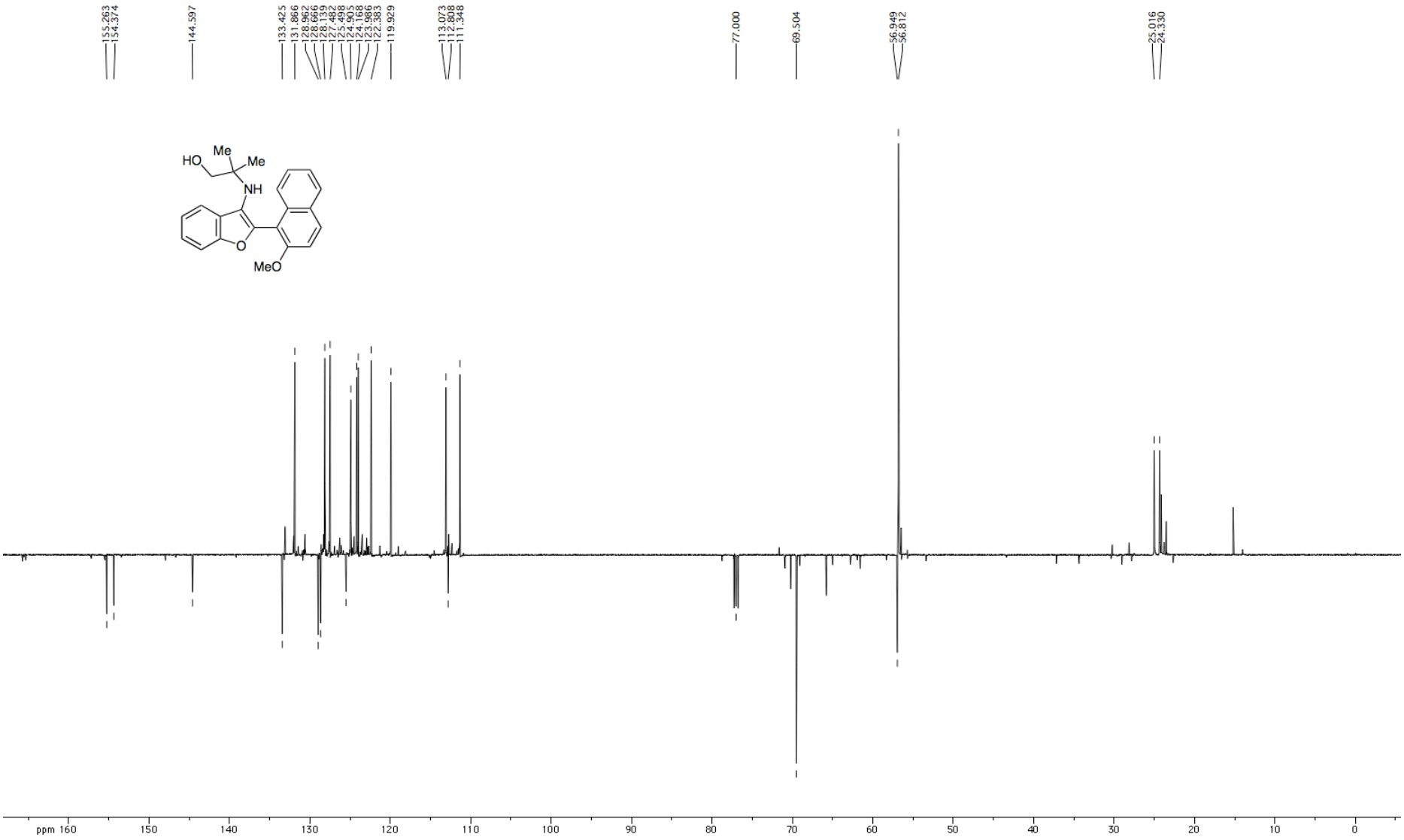
125 MHz DEPTQ ^{13}C NMR Spectrum of 2-((2-(2-Methoxyphenyl)benzofuran-3-yl)amino)-2-methylpropan-1-ol 6d



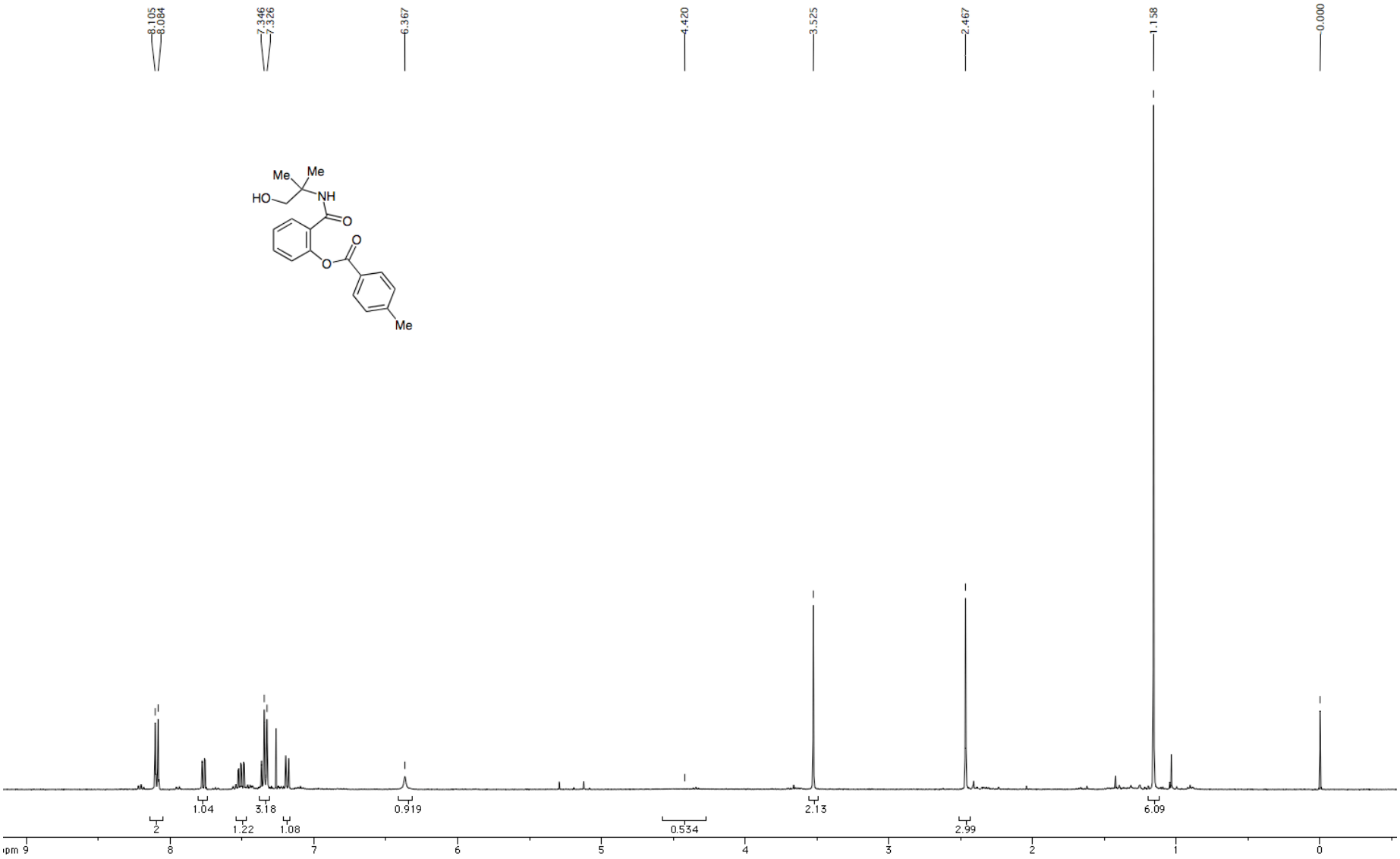
400 MHz ^{1}H NMR Spectrum of 2-((2-(2-Methoxynaphthalen-1-yl)benzofuran-3-yl)amino)-2-methylpropan-1-ol 6e



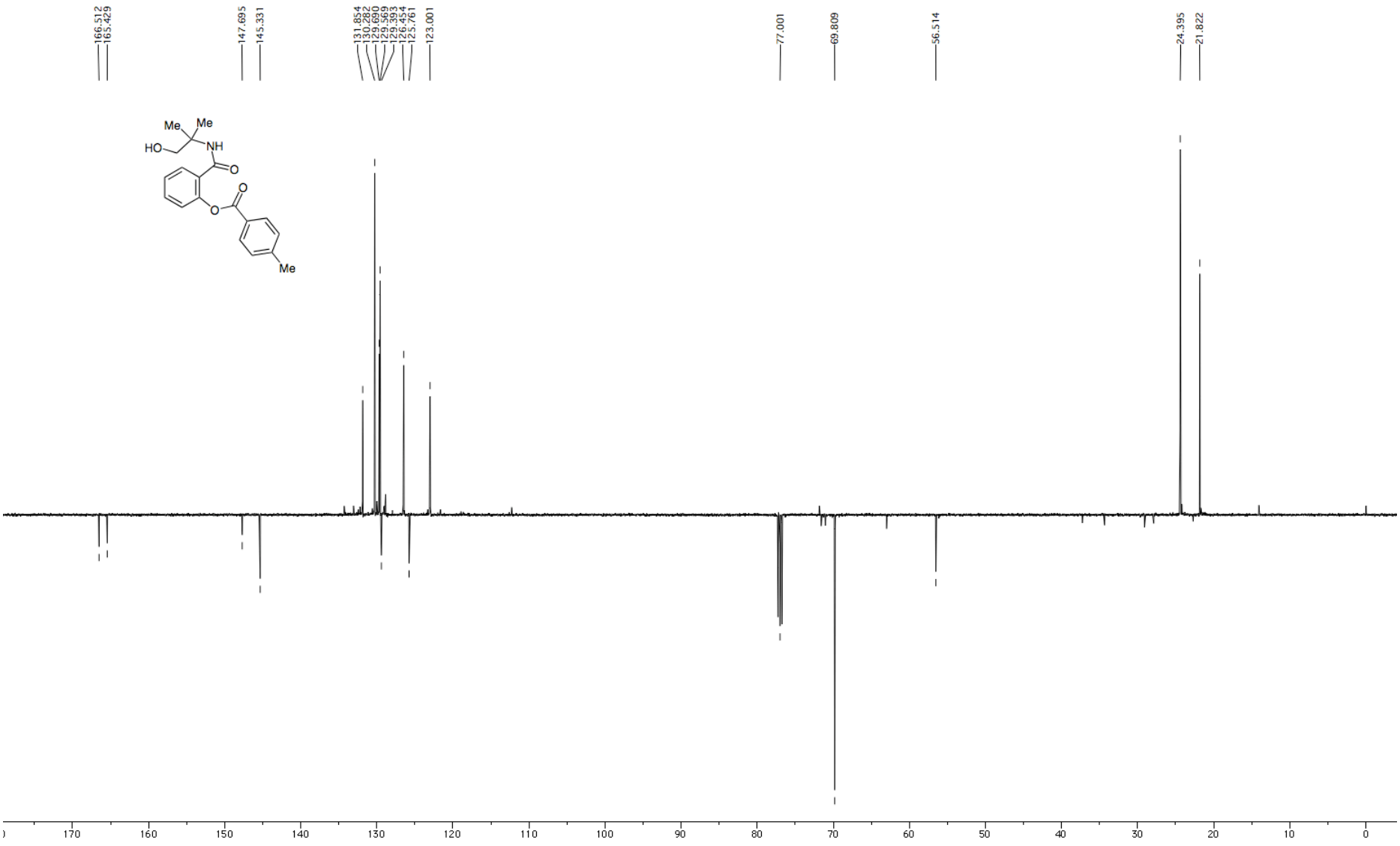
125 MHz DEPTQ ^{13}C NMR Spectrum of 2-((2-(2-Methoxynaphthalen-1-yl)benzofuran-3-yl)amino)-2-methylpropan-1-ol 6e



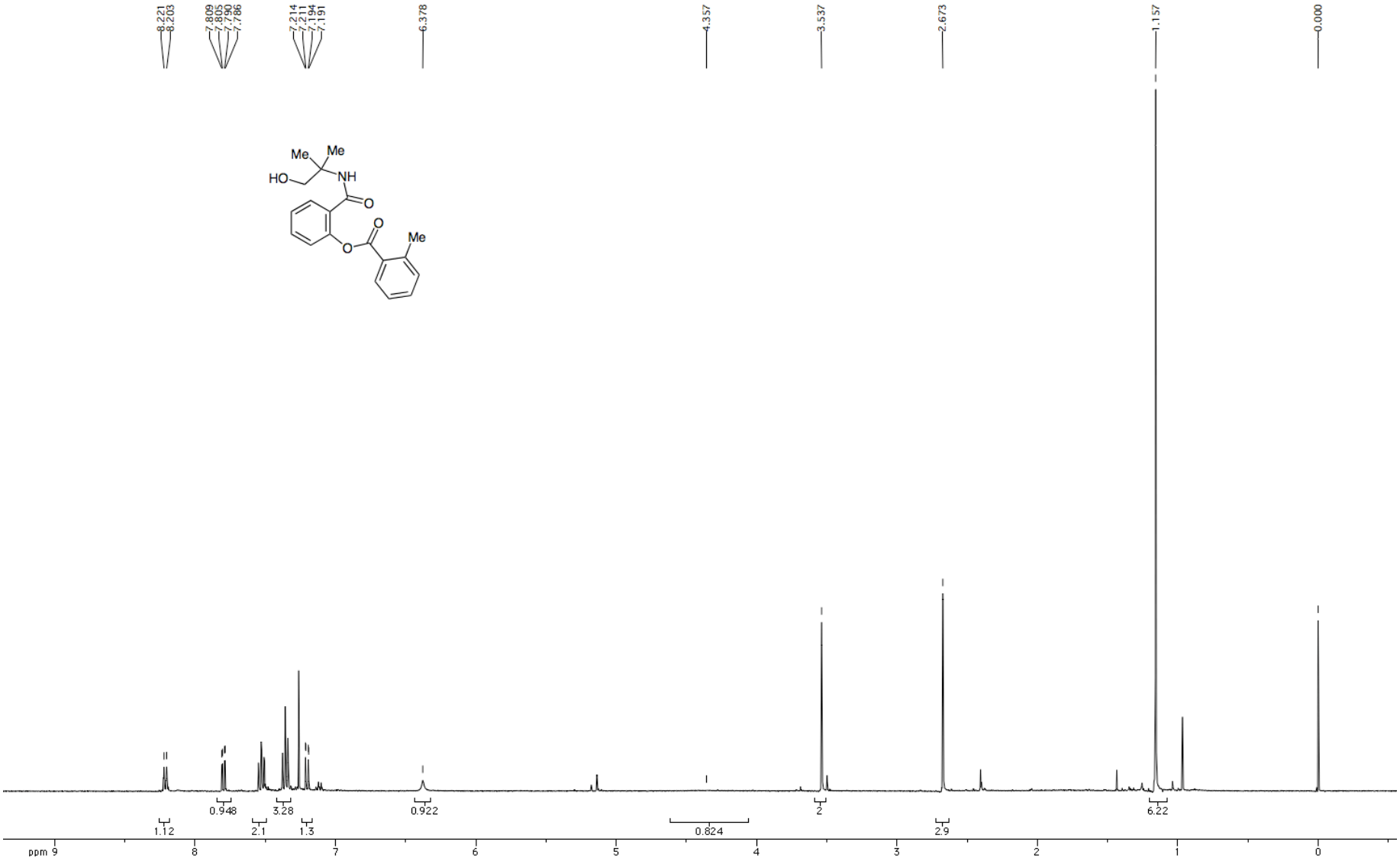
400 MHz ^{1}H NMR Spectrum of 2-((1-Hydroxy-2-methylpropan-2-yl)carbamoyl)phenyl 4-methylbenzoate 7a



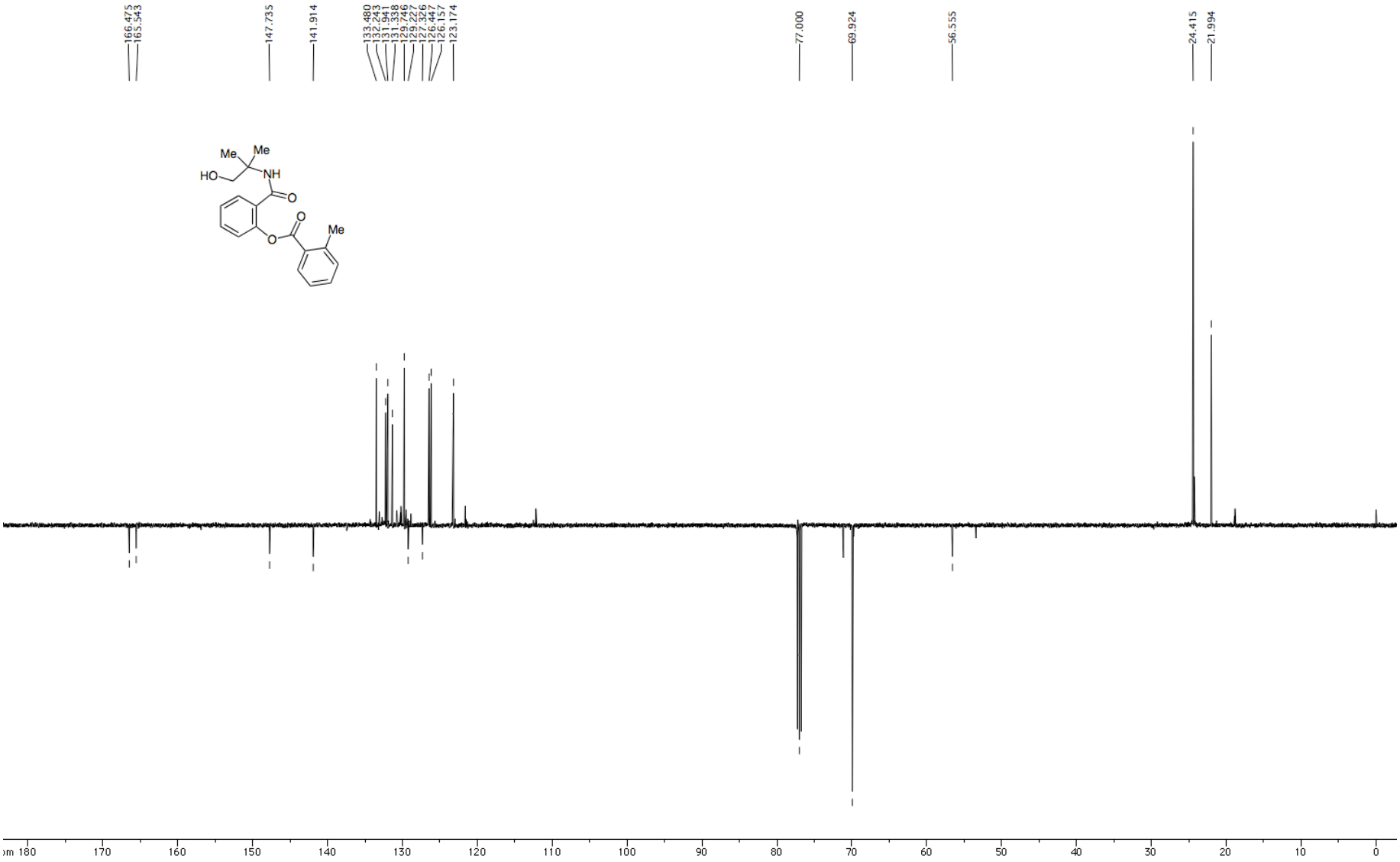
125 MHz DEPTQ ^{13}C NMR Spectrum of 2-((1-Hydroxy-2-methylpropan-2-yl)carbamoyl)phenyl 4-methylbenzoate 7a



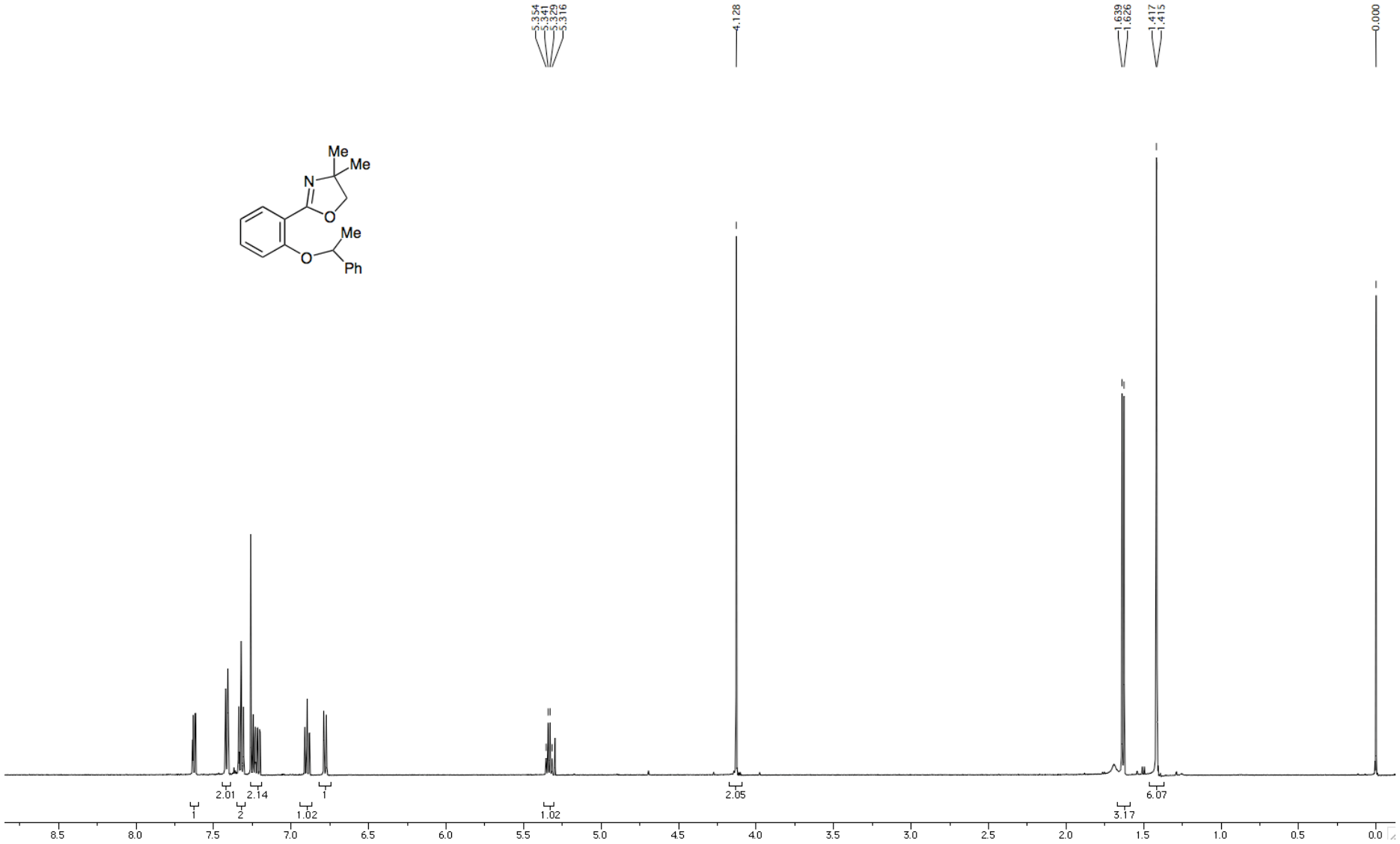
400 MHz ^{1}H NMR Spectrum of 2-((1-Hydroxy-2-methylpropan-2-yl)carbamoyl)phenyl 2-methylbenzoate 7b



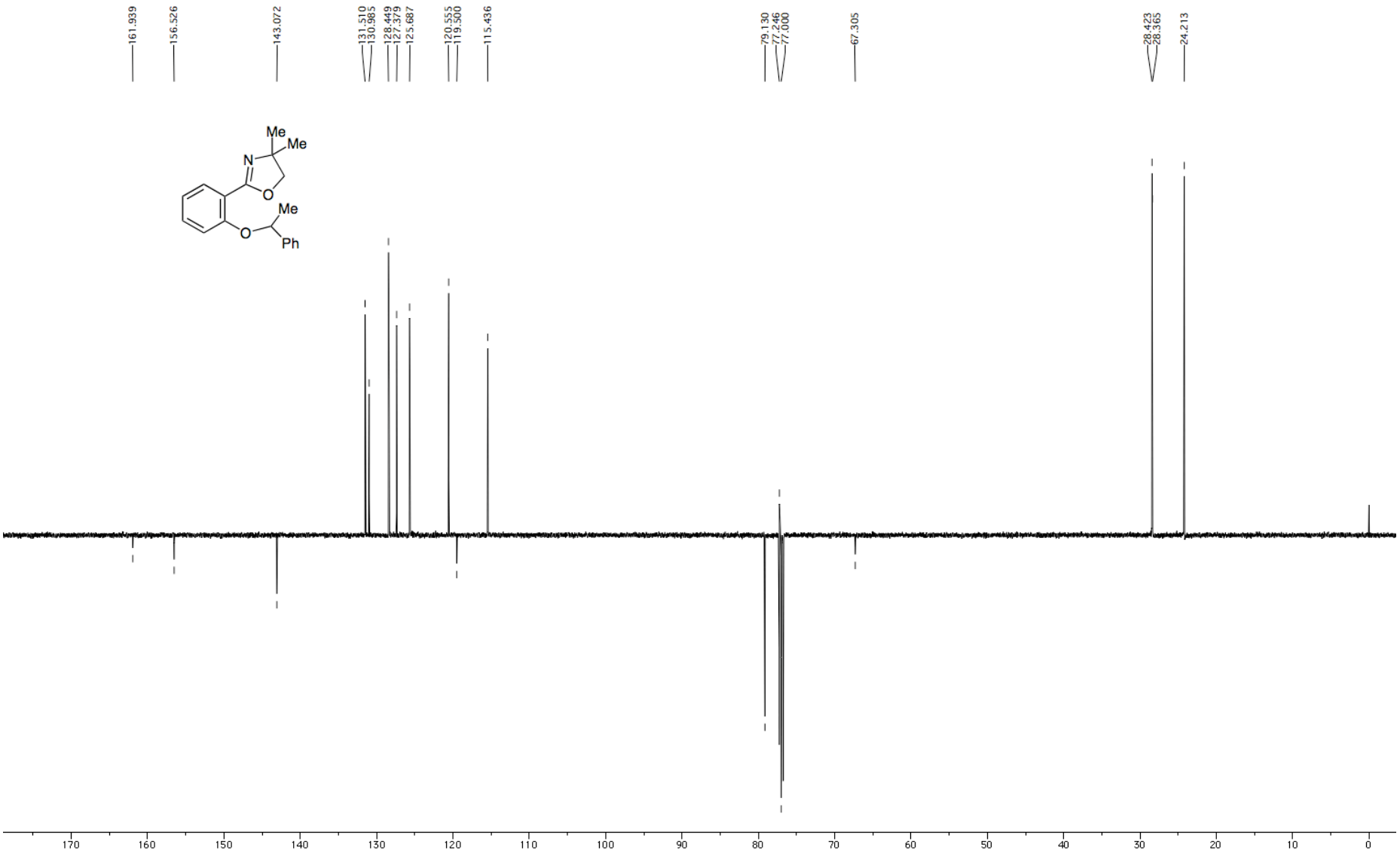
125 MHz DEPTQ ^{13}C NMR Spectrum of 2-((1-Hydroxy-2-methylpropan-2-yl)carbamoyl)phenyl 2-methylbenzoate 7b



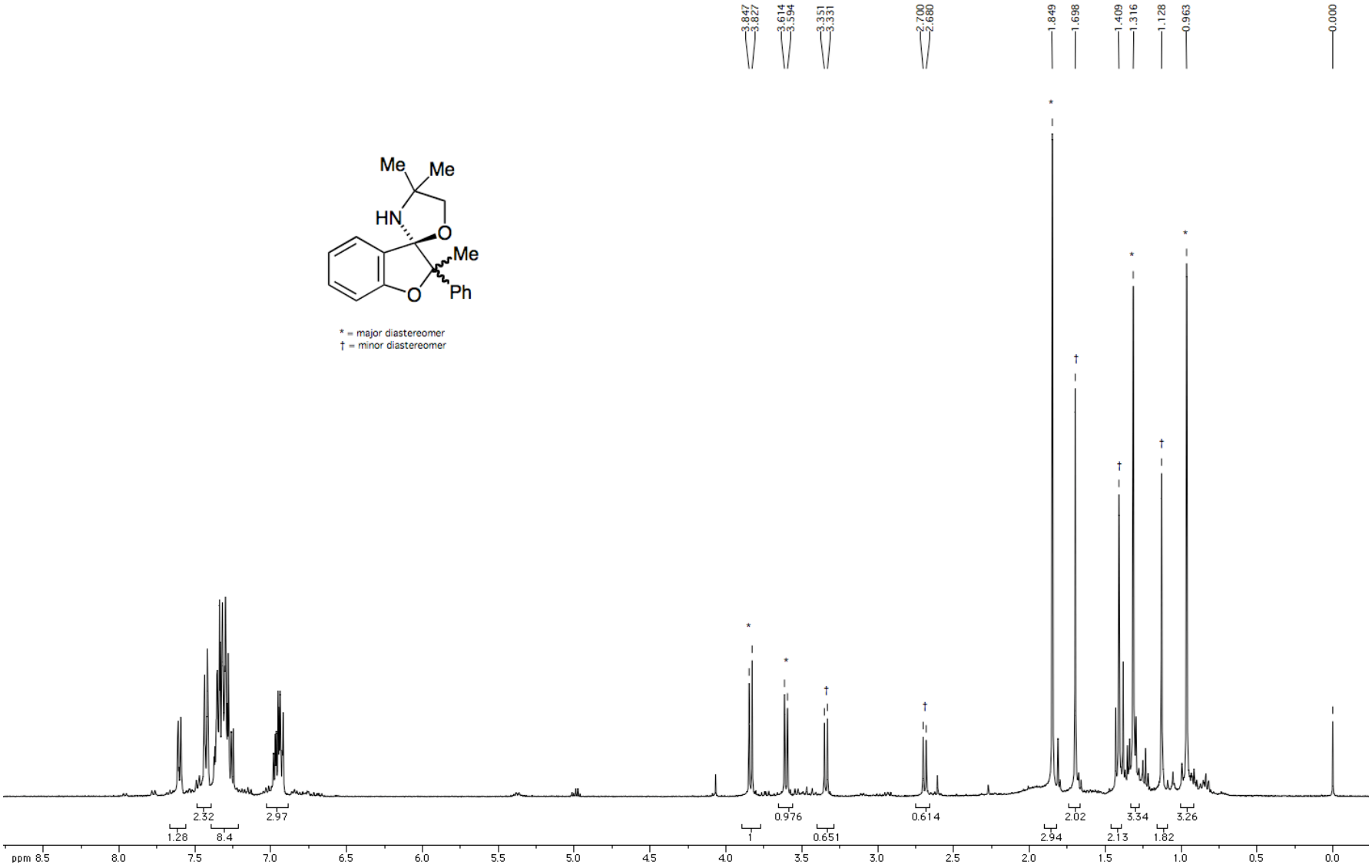
500 MHz ^{1}H NMR Spectrum of 4,4-Dimethyl-2-(2-(1-phenylethoxy)phenyl)-4,5-dihydrooxazole 8



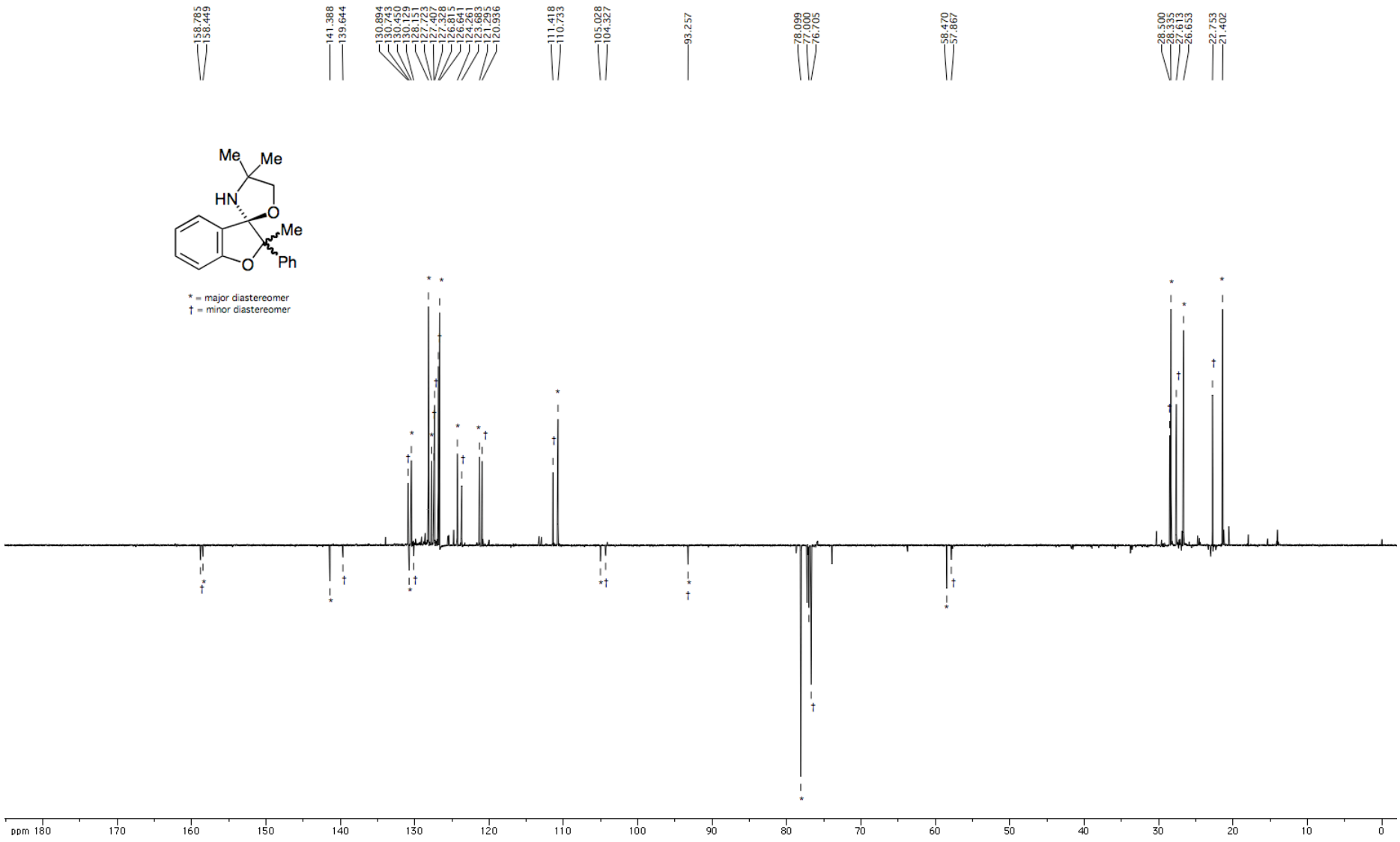
125 MHz DEPTQ ^{13}C NMR Spectrum of 4,4-Dimethyl-2-(2-(1-phenylethoxy)phenyl)-4,5-dihydrooxazole 8



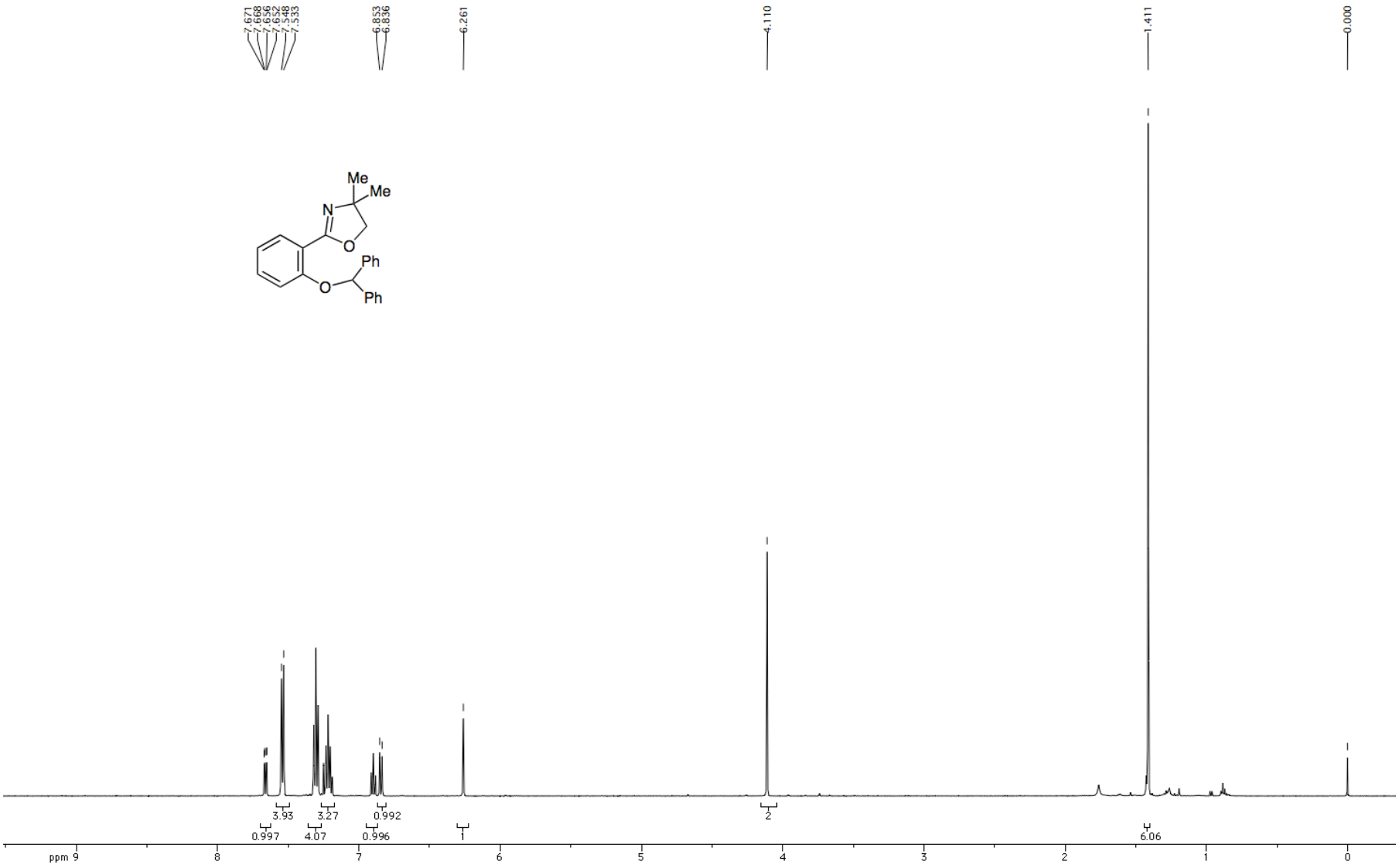
400 MHz ^{1}H NMR Spectrum of 2,4',4'-Trimethyl-2-phenyl-2*H*-spiro[benzofuran-3,2'-oxazolidine] 9



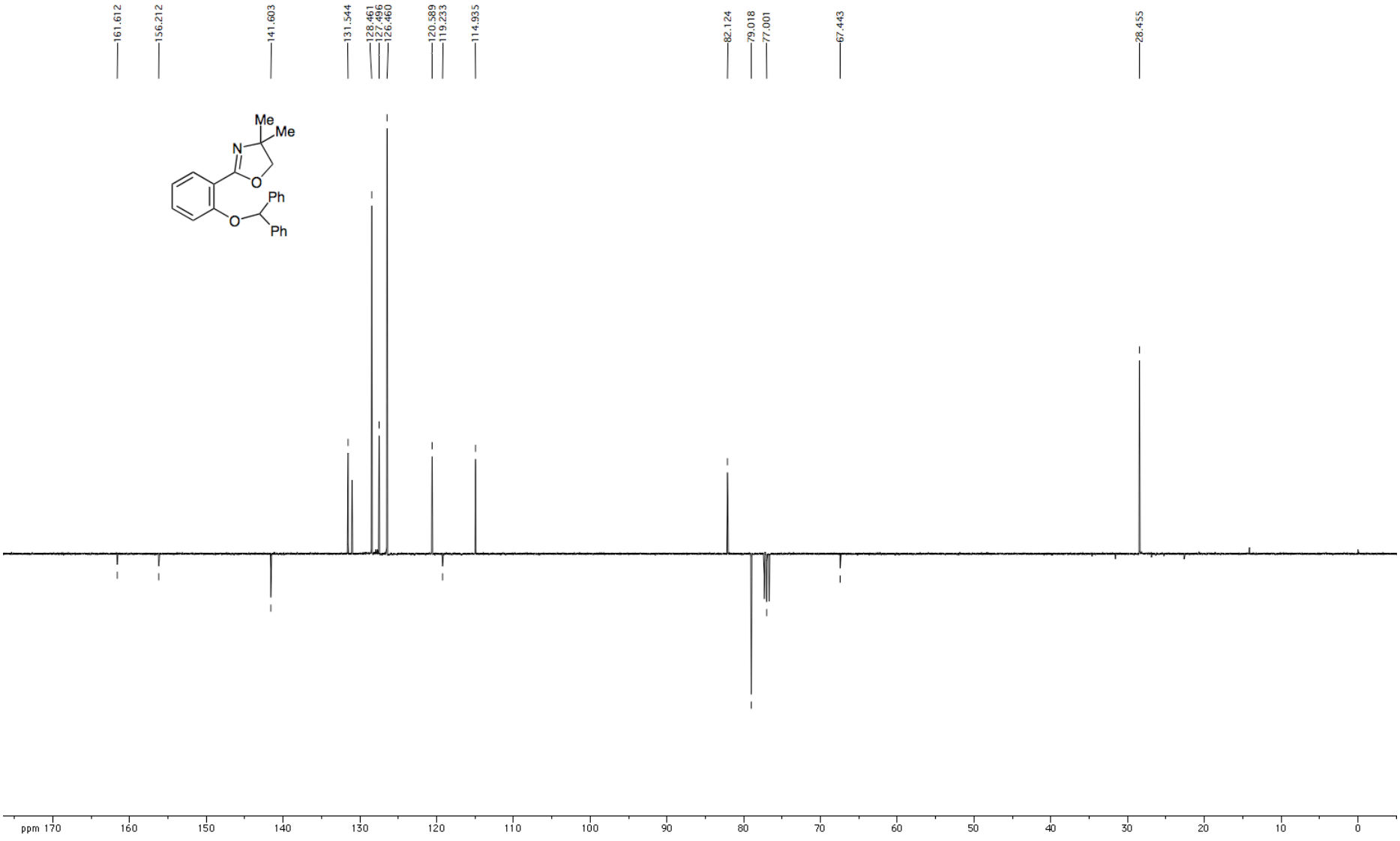
125 MHz DEPTQ ^{13}C NMR Spectrum of 2,4',4'-Trimethyl-2-phenyl-2*H*-spiro[benzofuran-3,2'-oxazolidine] 9



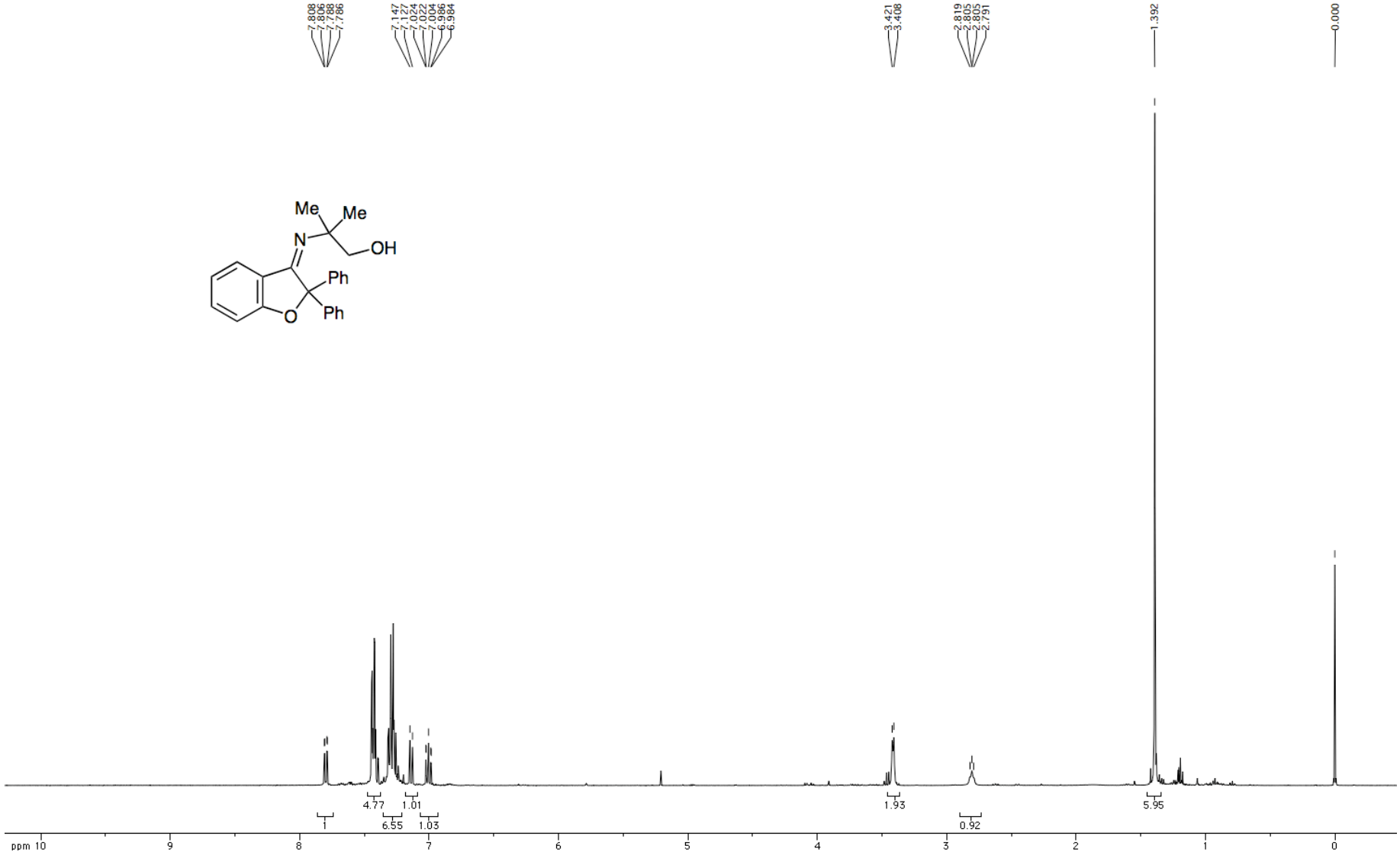
500 MHz ^{1}H NMR Spectrum of 2-(2-(Benzhydryloxy)phenyl)-4,4-dimethyl-4,5-dihydrooxazole 10



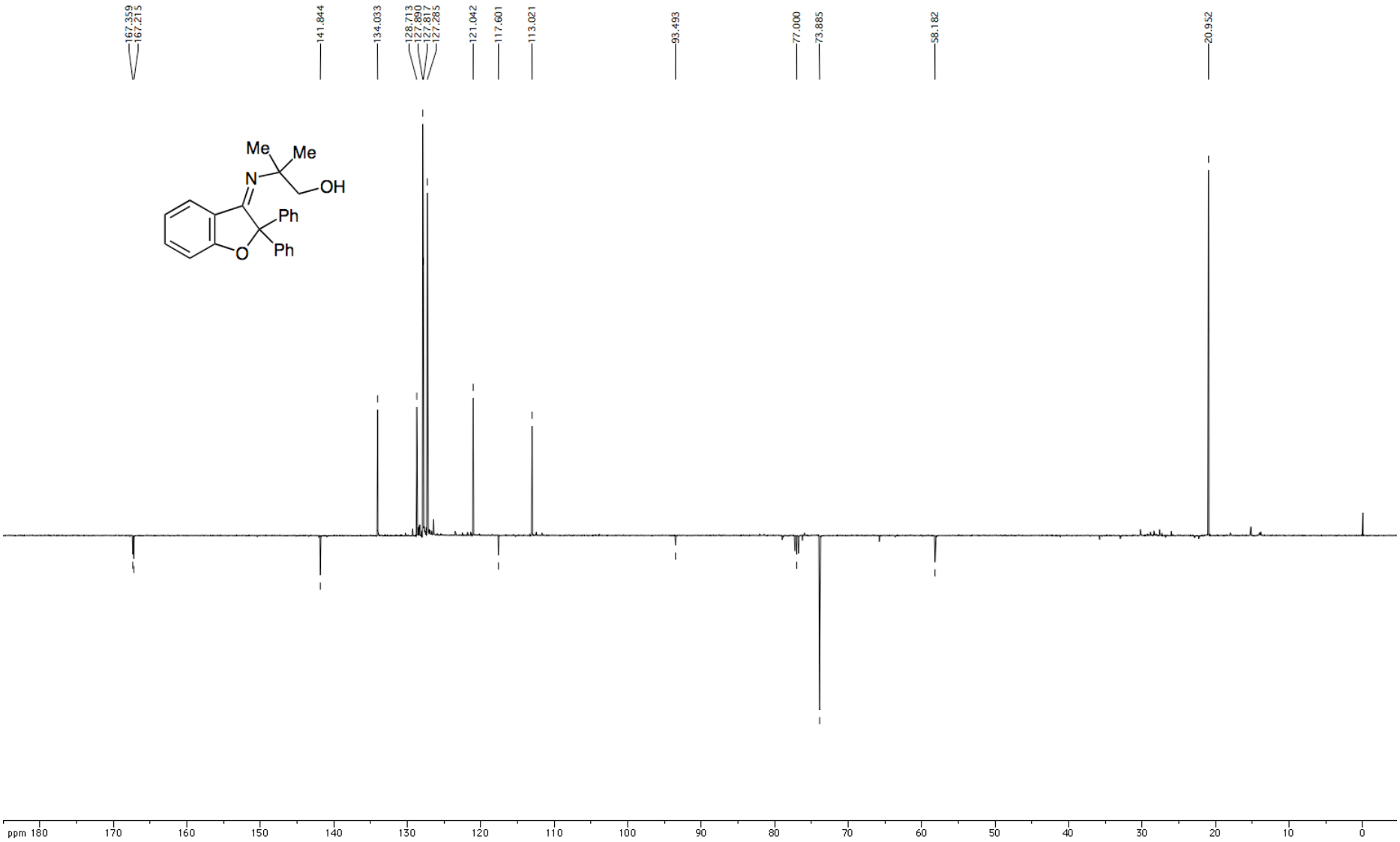
100 MHz DEPTQ ^{13}C NMR Spectrum of 2-(2-(Benzhydryloxy)phenyl)-4,4-dimethyl-4,5-dihydrooxazole 10



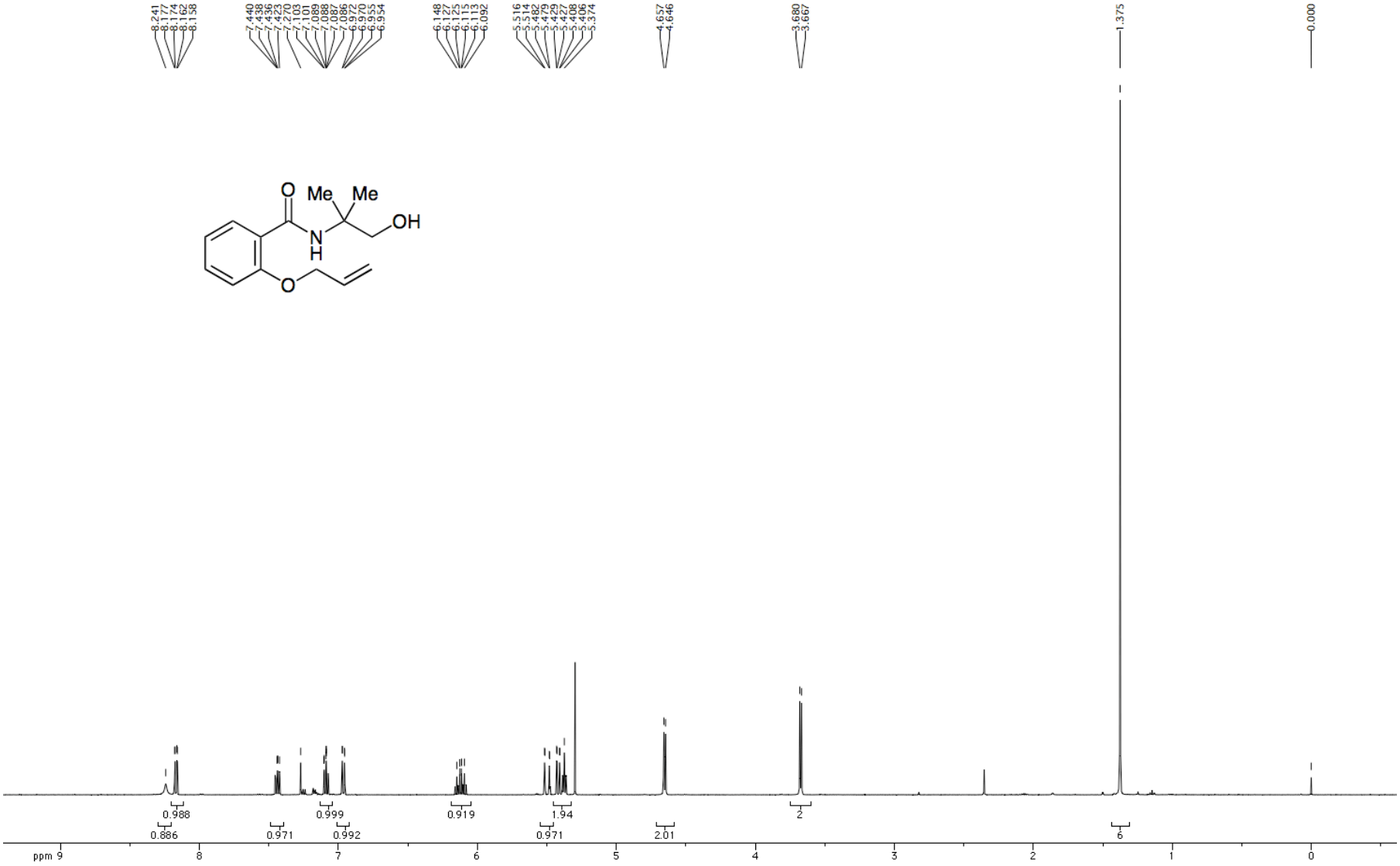
400 MHz ^{1}H NMR Spectrum of 2-((2,2-Diphenylbenzofuran-3(2*H*)-ylidene)amino)-2-methylpropan-1-ol 11



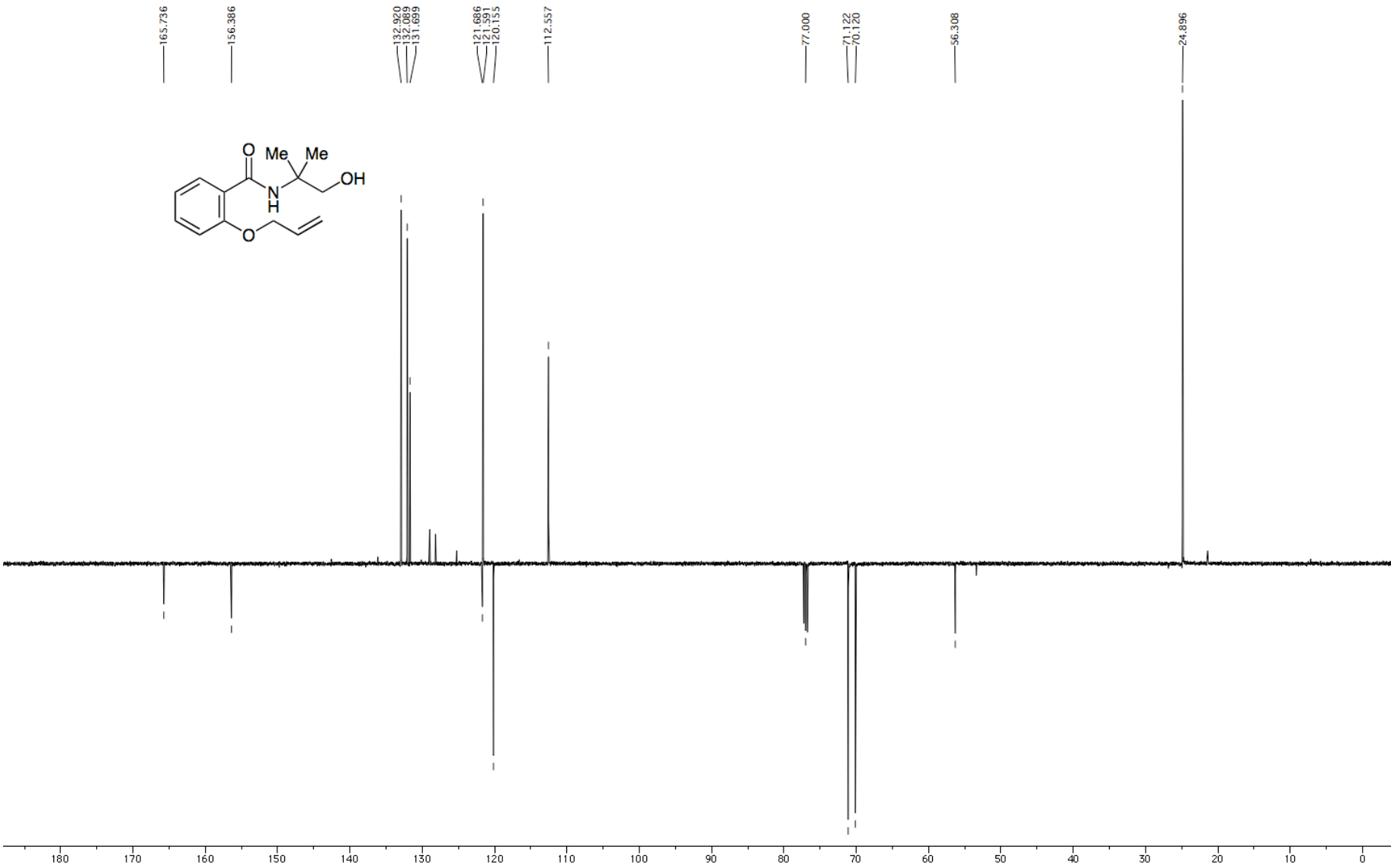
125 MHz DEPTQ ^{13}C NMR Spectrum of 2-((2,2-Diphenylbenzofuran-3(2*H*)-ylidene)amino)-2-methylpropan-1-ol 11



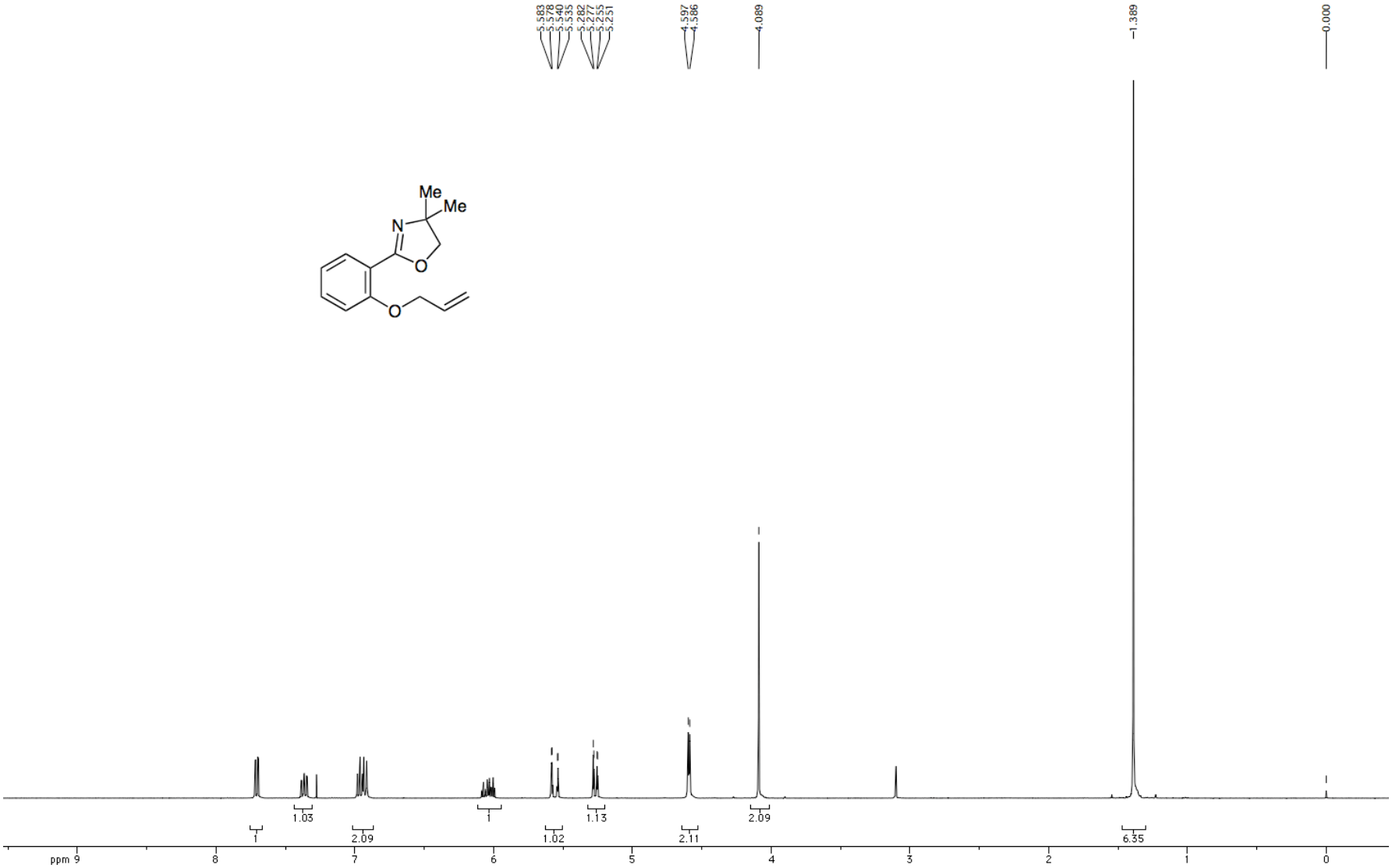
500 MHz ^{1}H NMR Spectrum of 2-(Allyloxy)-*N*-(1-hydroxy-2-methylpropan-2-yl)benzamide E



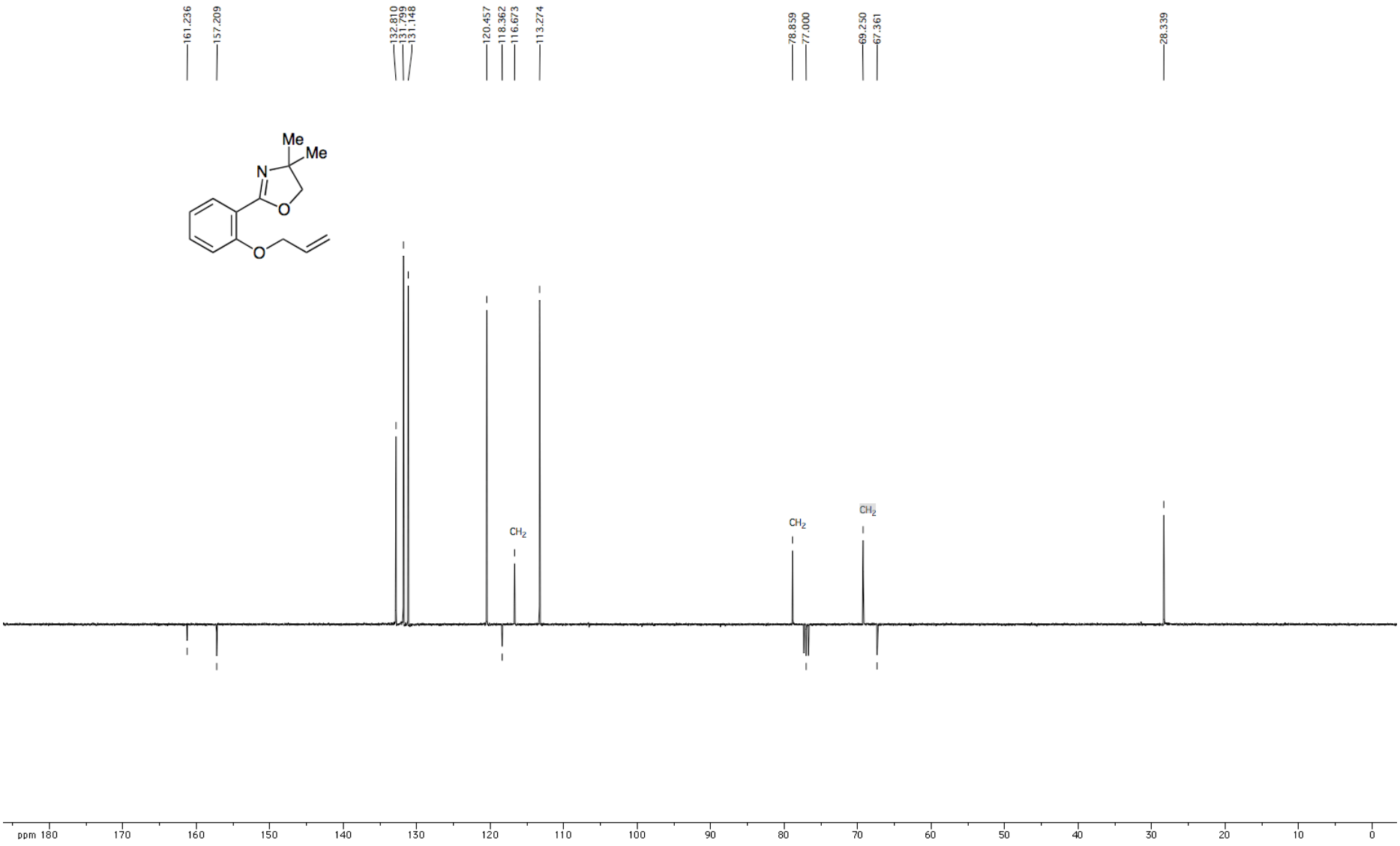
125 MHz DEPTQ ^{13}C NMR Spectrum of 2-(Allyloxy)-*N*-(1-hydroxy-2-methylpropan-2-yl)benzamide E



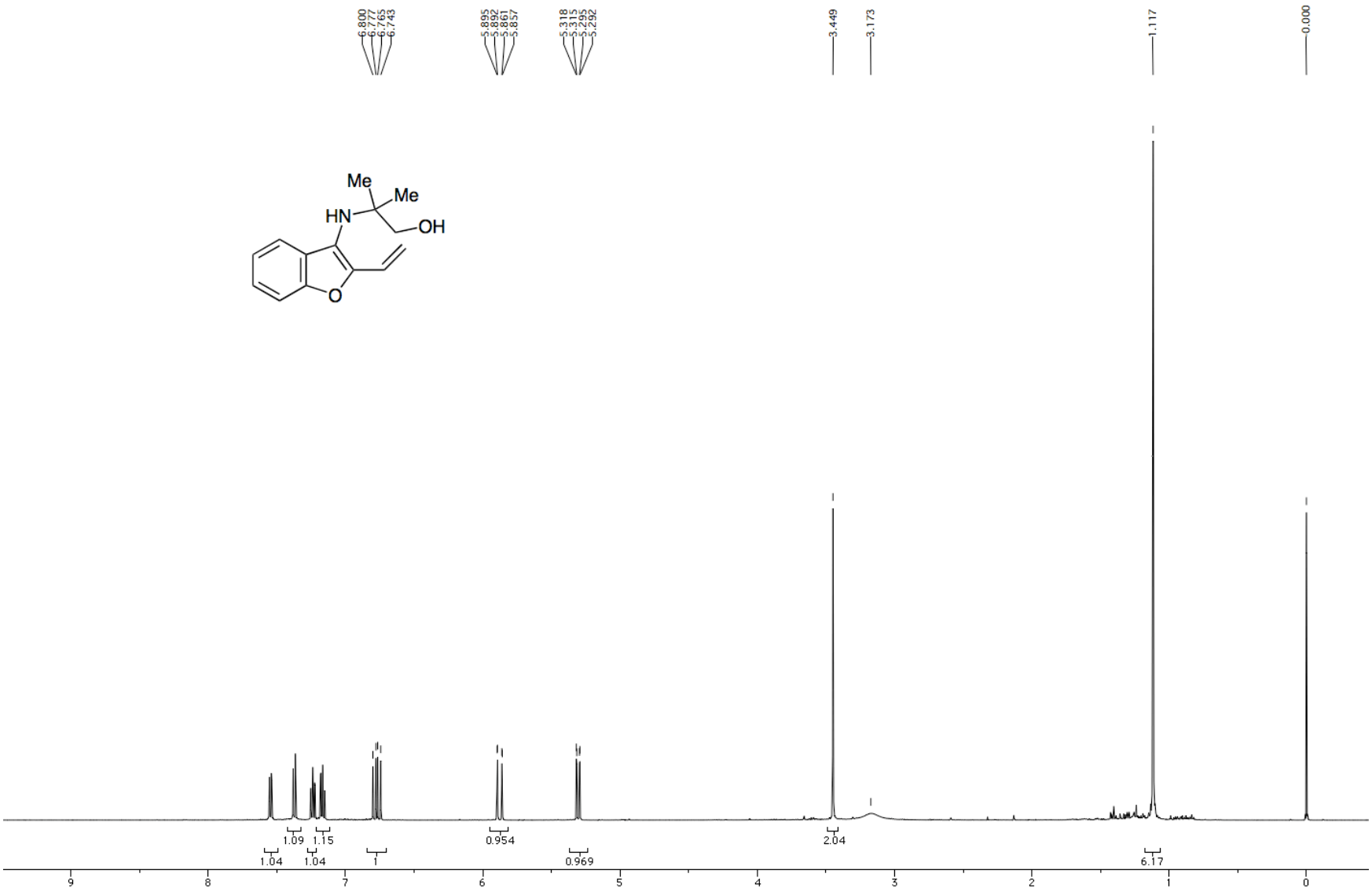
400 MHz ^{1}H NMR Spectrum of 2-(2-(Allyloxy)phenyl)-4,4-dimethyl-4,5-dihydrooxazole 12



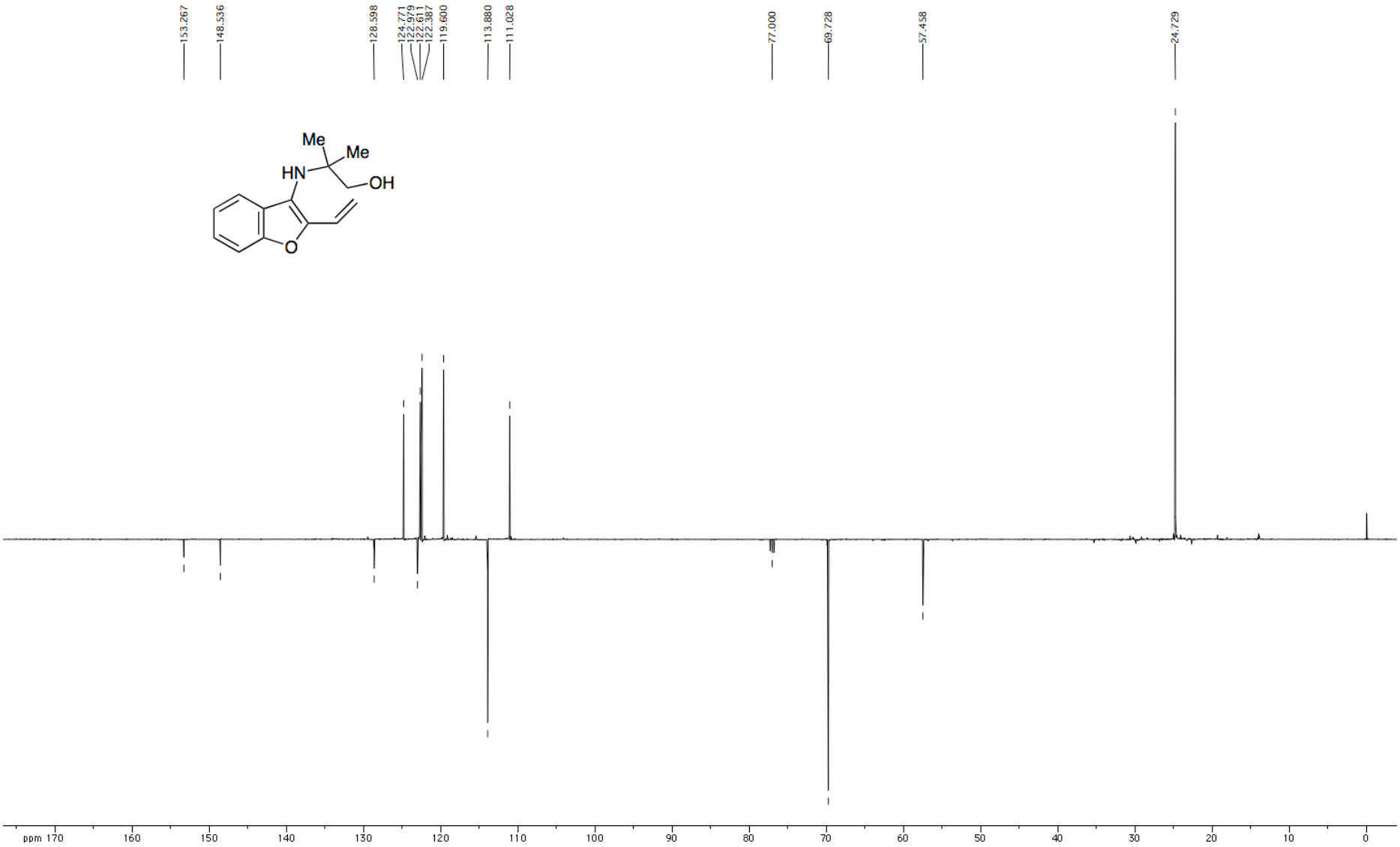
100 MHz DEPTQ ^{13}C NMR Spectrum of 2-(2-(Allyloxy)phenyl)-4,4-dimethyl-4,5-dihydrooxazole 12



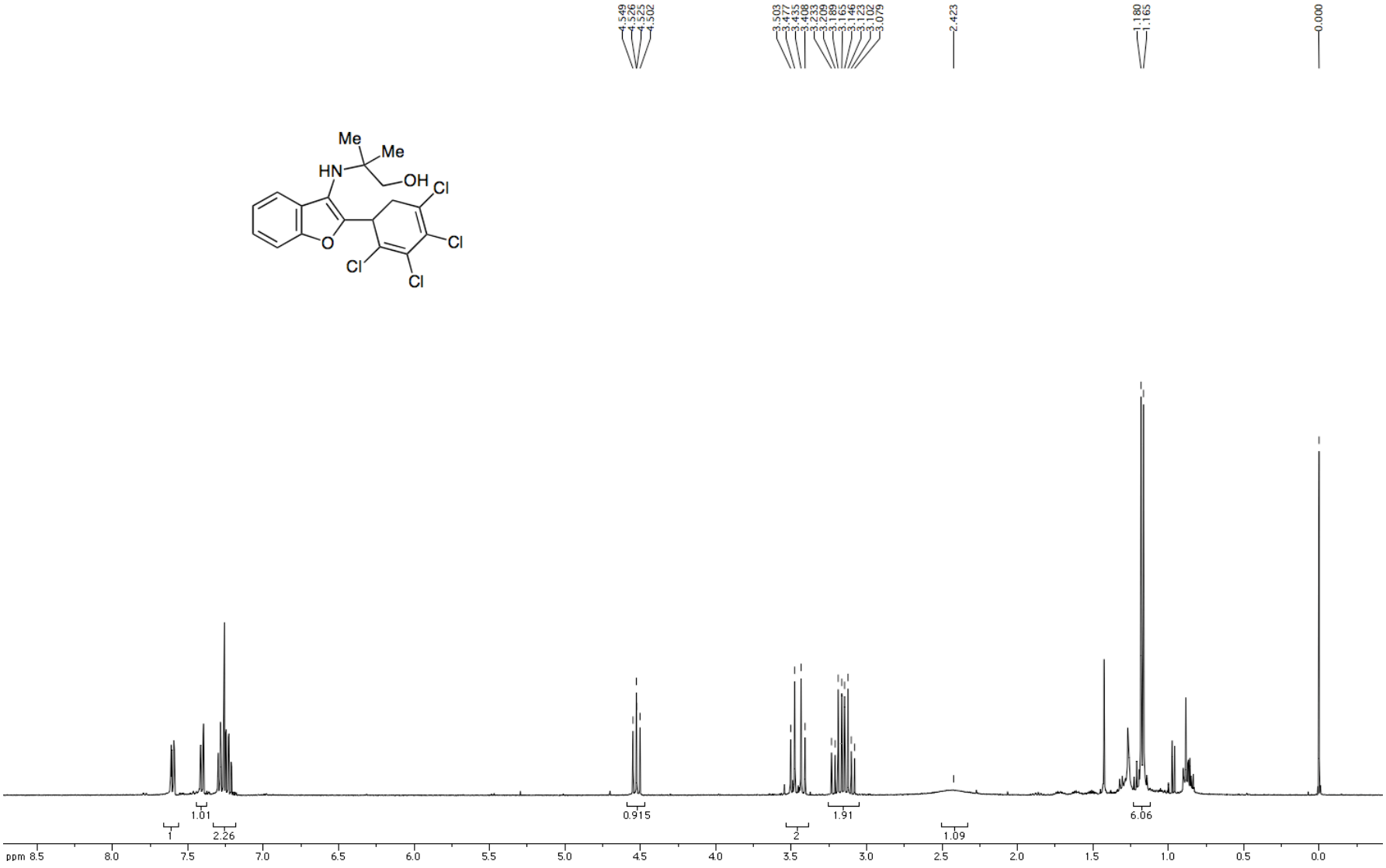
500 MHz ^{1}H NMR Spectrum of 2-Methyl-2-((2-vinylbenzofuran-3-yl)amino)propan-1-ol 13



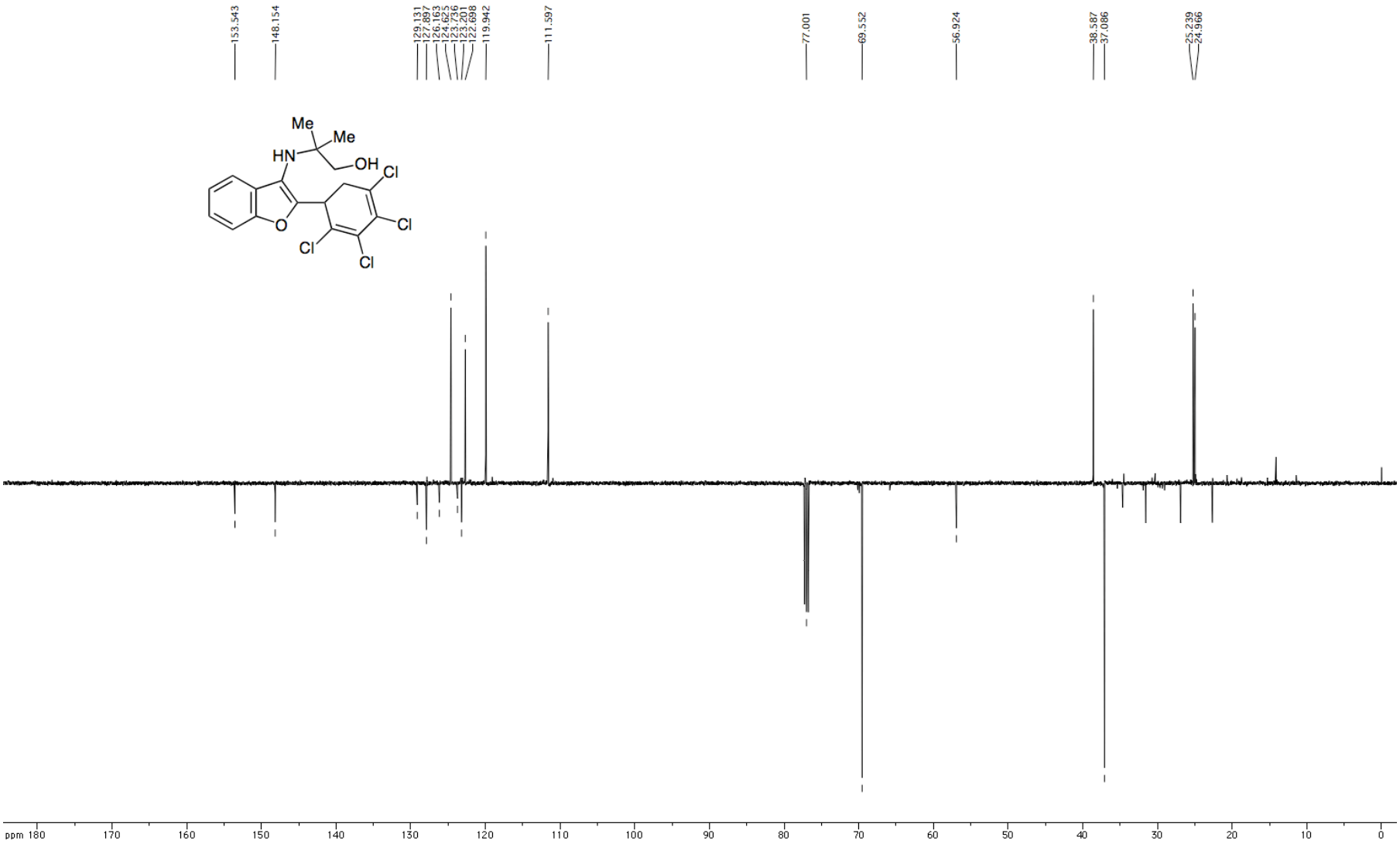
125 MHz DEPTQ ^{13}C NMR Spectrum of 2-Methyl-2-((2-vinylbenzofuran-3-yl)amino)propan-1-ol 13



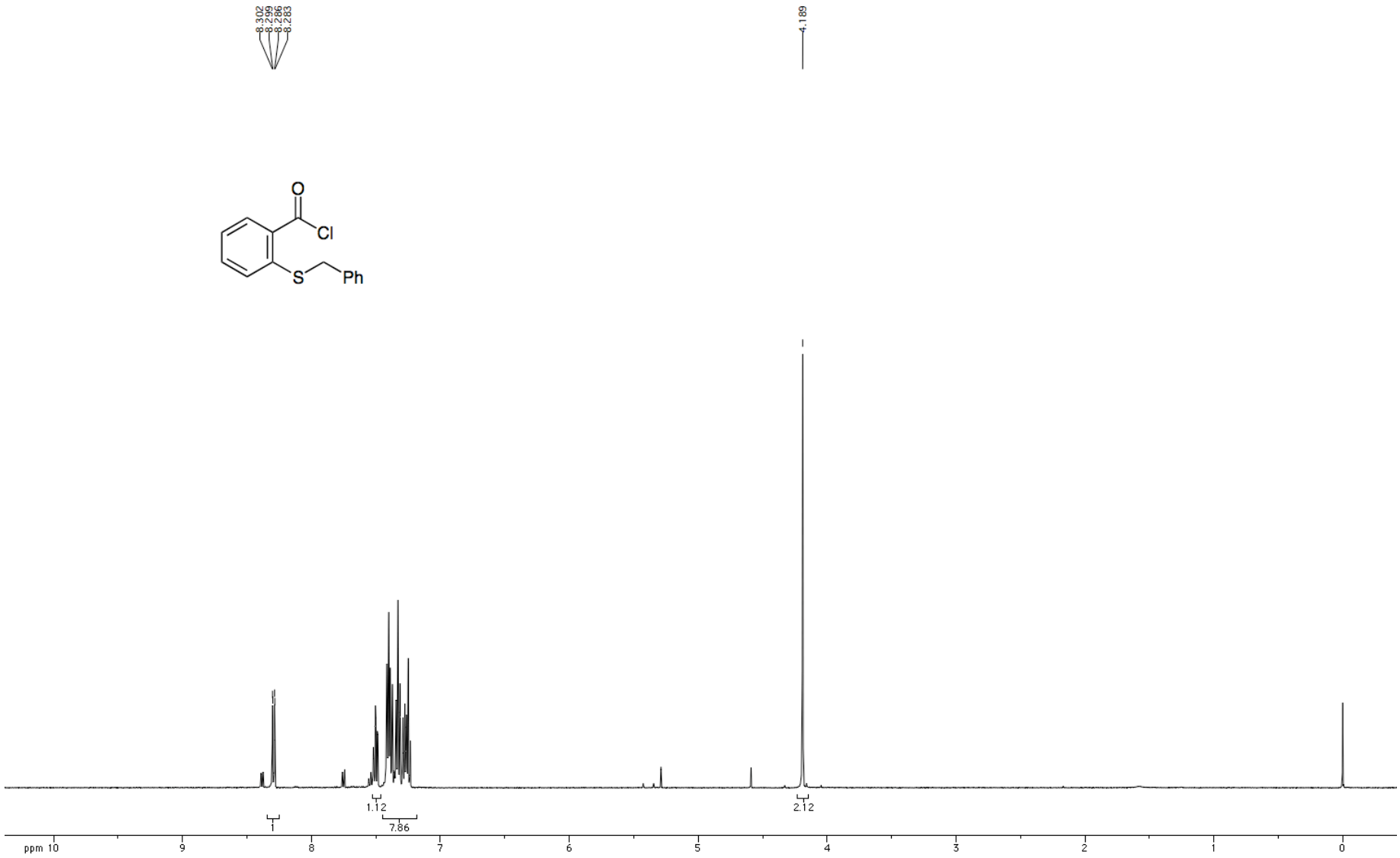
400 MHz ^{1}H NMR Spectrum of 2-Methyl-2-((2-(2,3,4,5-tetrachlorocyclohexa-2,4-dien-1-yl)benzofuran-3-yl)amino)propan-1-ol 14



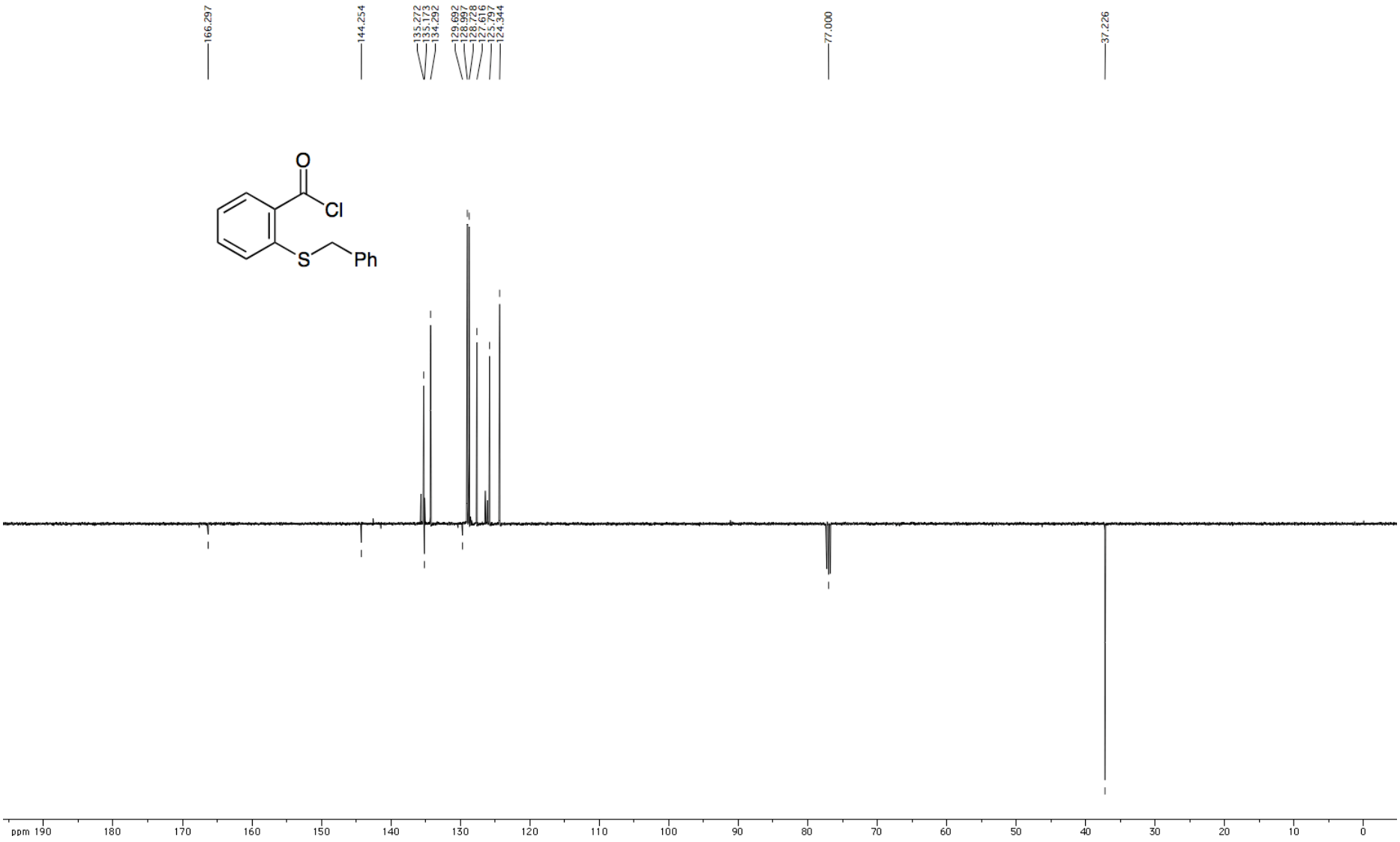
125 MHz DEPTQ ^{13}C NMR Spectrum of 2-Methyl-2-((2-(2,3,4,5-tetrachlorocyclohexa-2,4-dien-1-yl)benzofuran-3-yl)amino)propan-1-ol 14



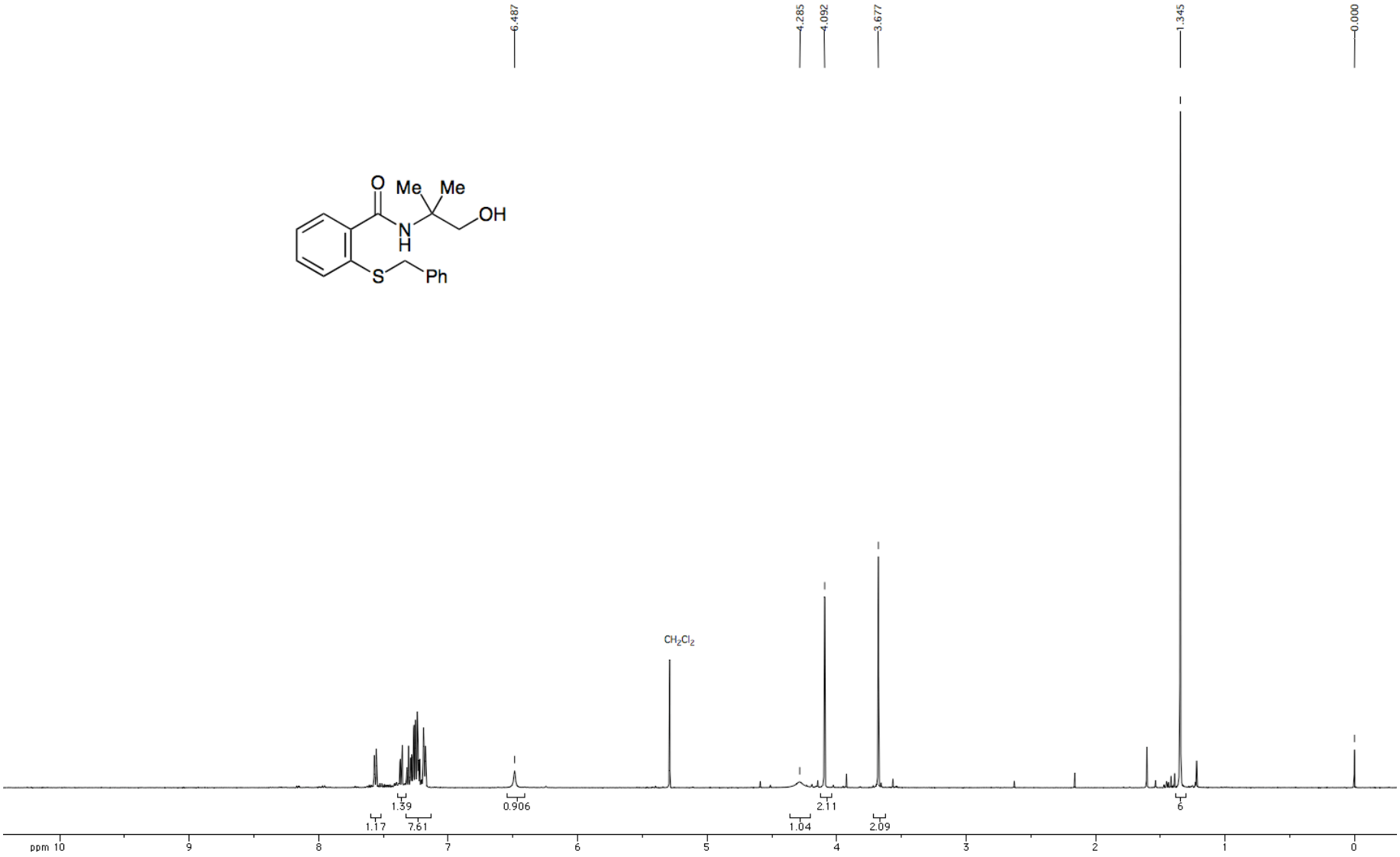
500 MHz ^{1}H NMR Spectrum of 2-(Benzylthio)benzoyl chloride F



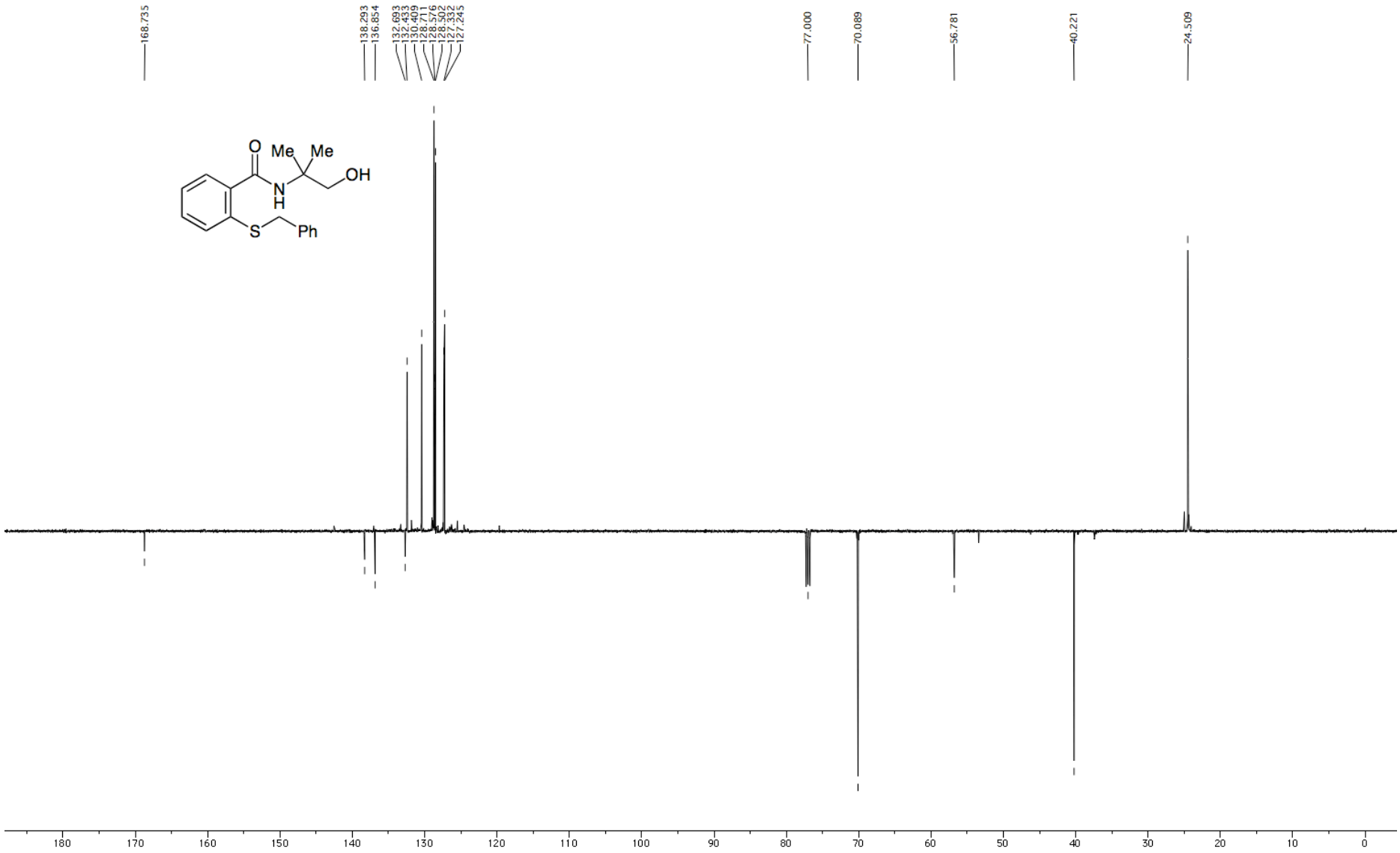
125 MHz DEPTQ ^{13}C NMR Spectrum of 2-(Benzylthio)benzoyl chloride F



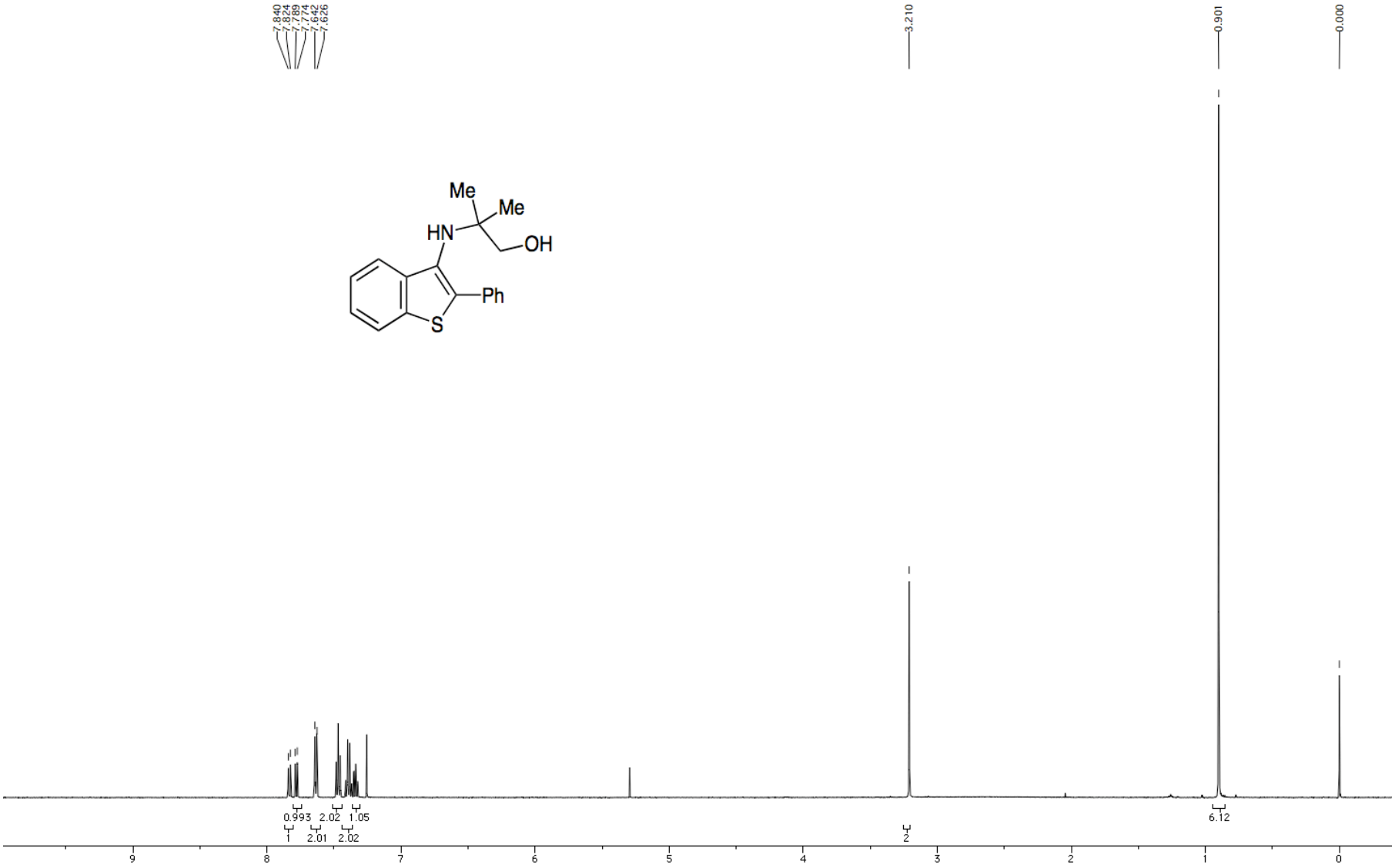
500 MHz ^{1}H NMR Spectrum of 2-(Benzylthio)-*N*-(1-hydroxy-2-methylpropan-2-yl)benzamide G



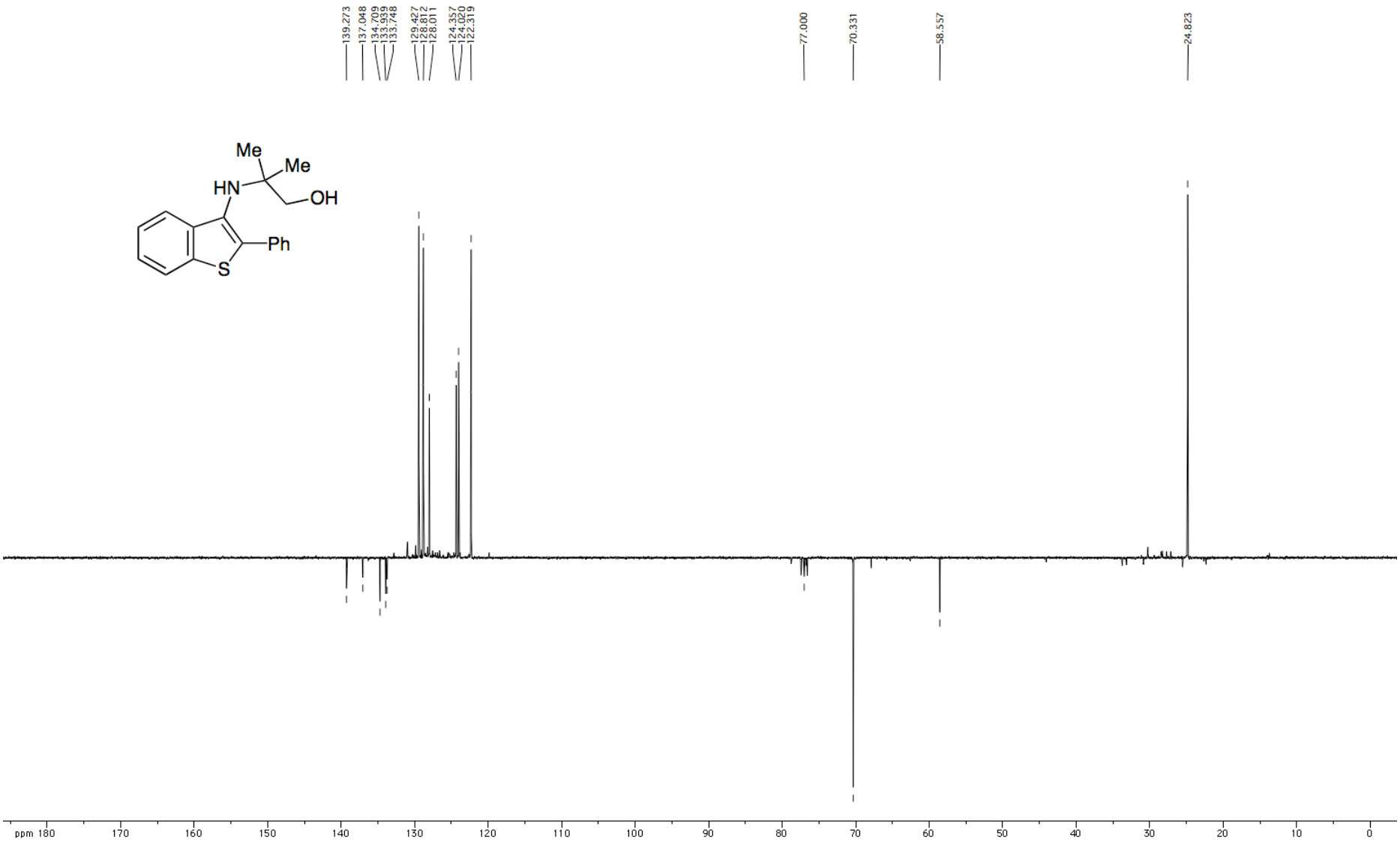
125 MHz DEPTQ ^{13}C NMR Spectrum of 2-(Benzylthio)-*N*-(1-hydroxy-2-methylpropan-2-yl)benzamide G



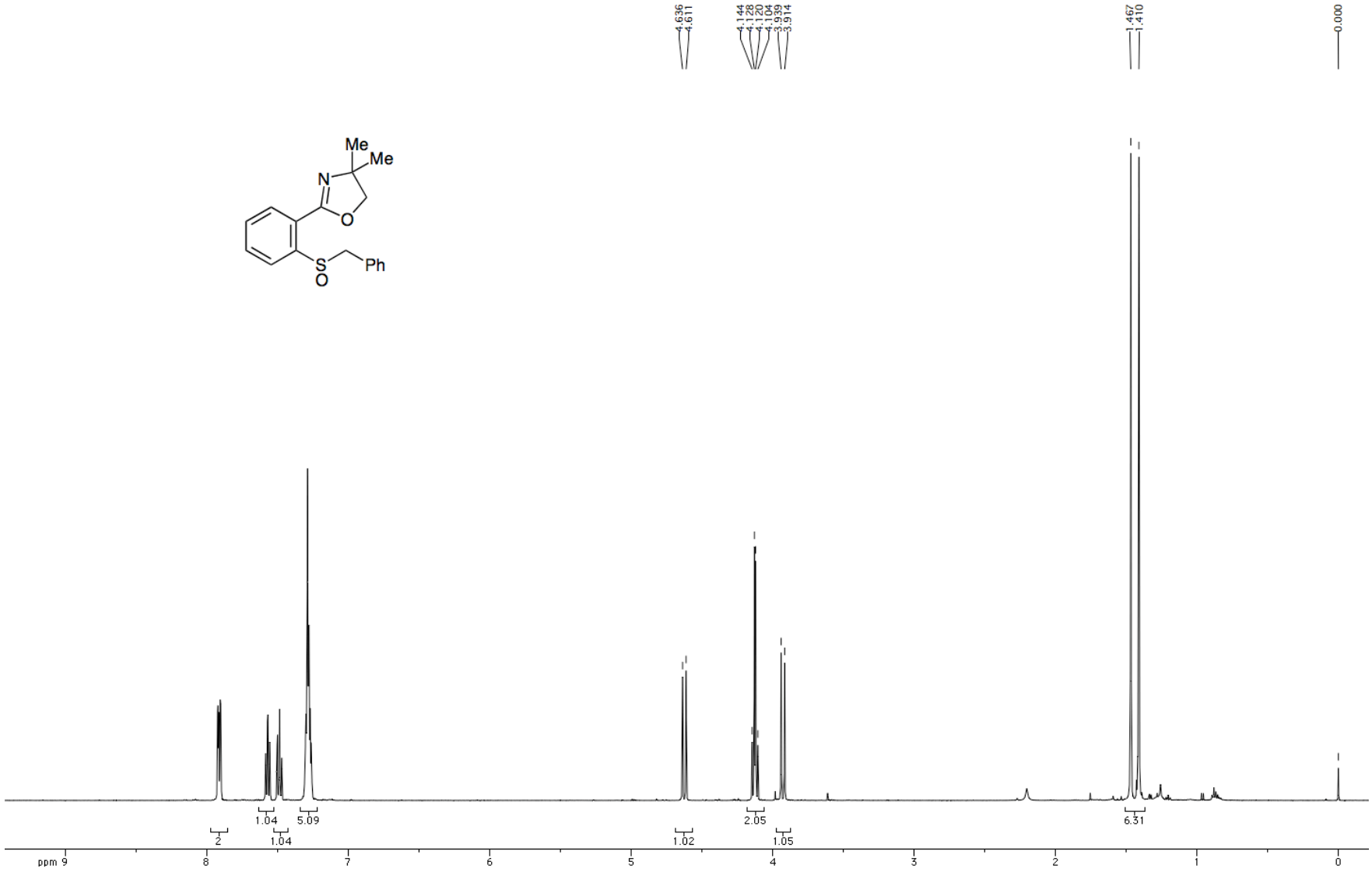
500 MHz ^{1}H NMR Spectrum of 2-Methyl-2-((2-phenylbenzo[*b*]thiophen-3-yl)amino)propan-1-ol 16



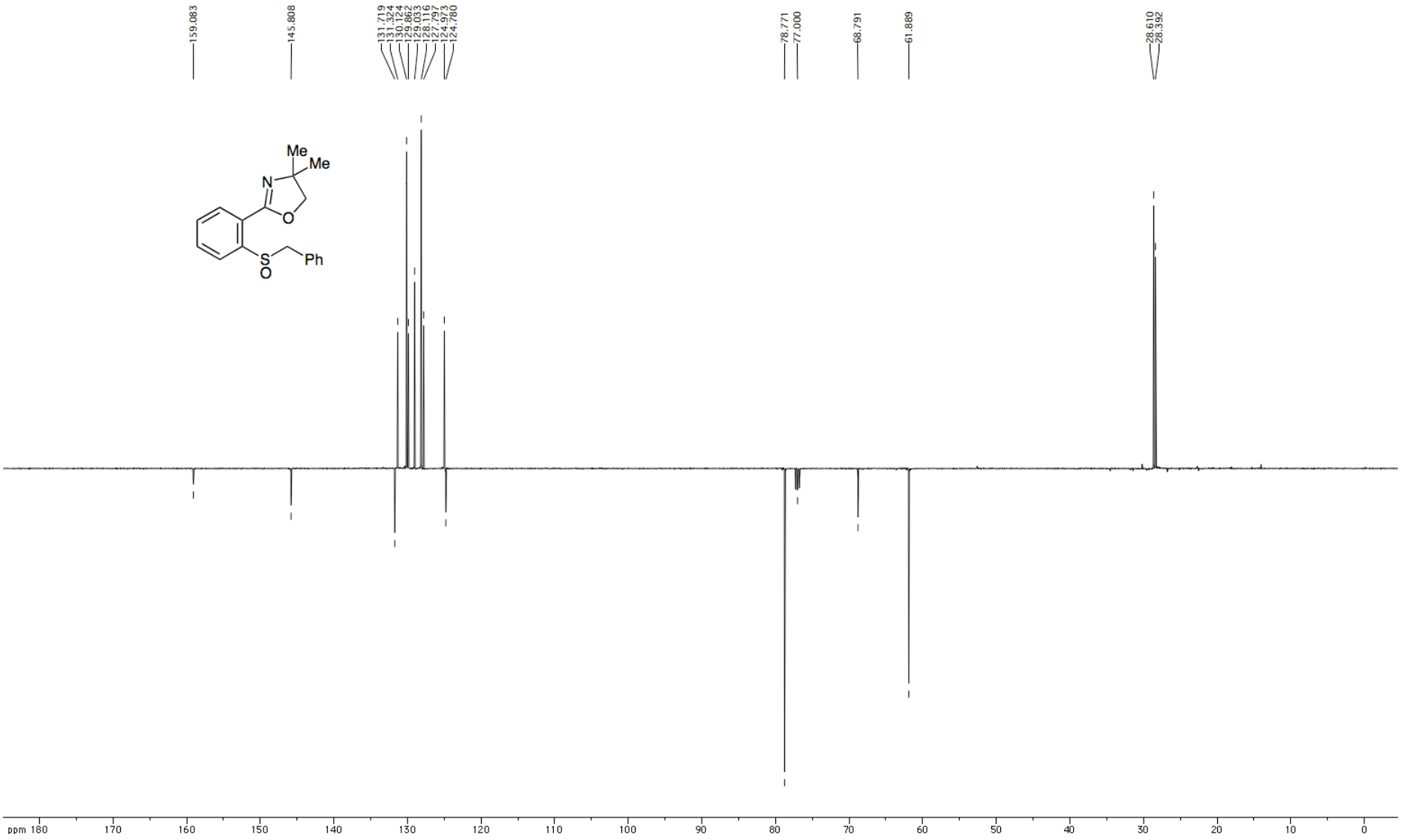
75 MHz DEPTQ ^{13}C NMR Spectrum of 2-Methyl-2-((2-phenylbenzo[*b*]thiophen-3-yl)amino)propan-1-ol 16



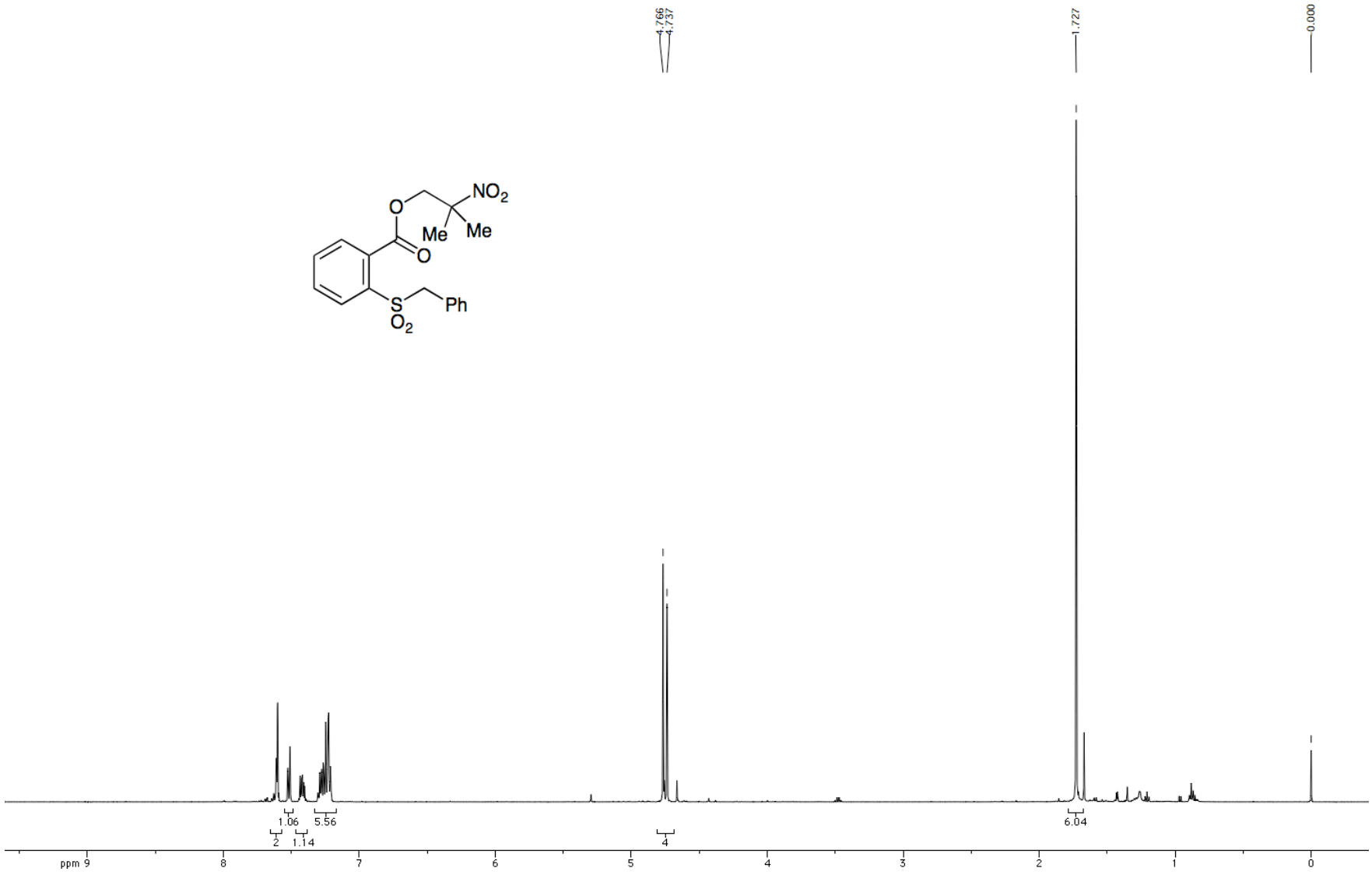
500 MHz ^{1}H NMR Spectrum of 2-(2-(Benzylsulfinyl)phenyl)-4,4-dimethyl-4,5-dihydrooxazole 17



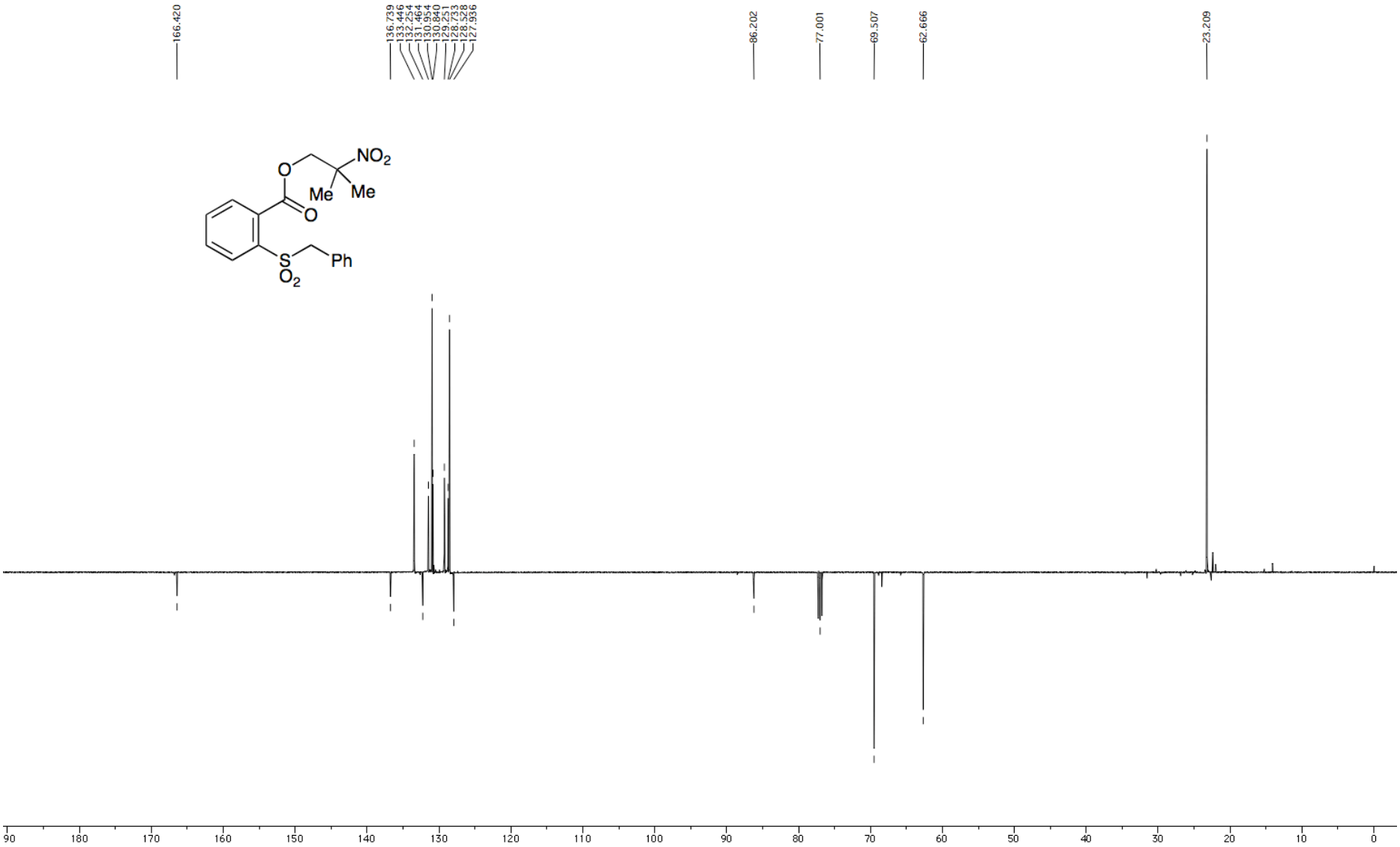
125 MHz DEPTQ ^{13}C NMR Spectrum of 2-(2-(Benzylsulfinyl)phenyl)-4,4-dimethyl-4,5-dihydrooxazole 17



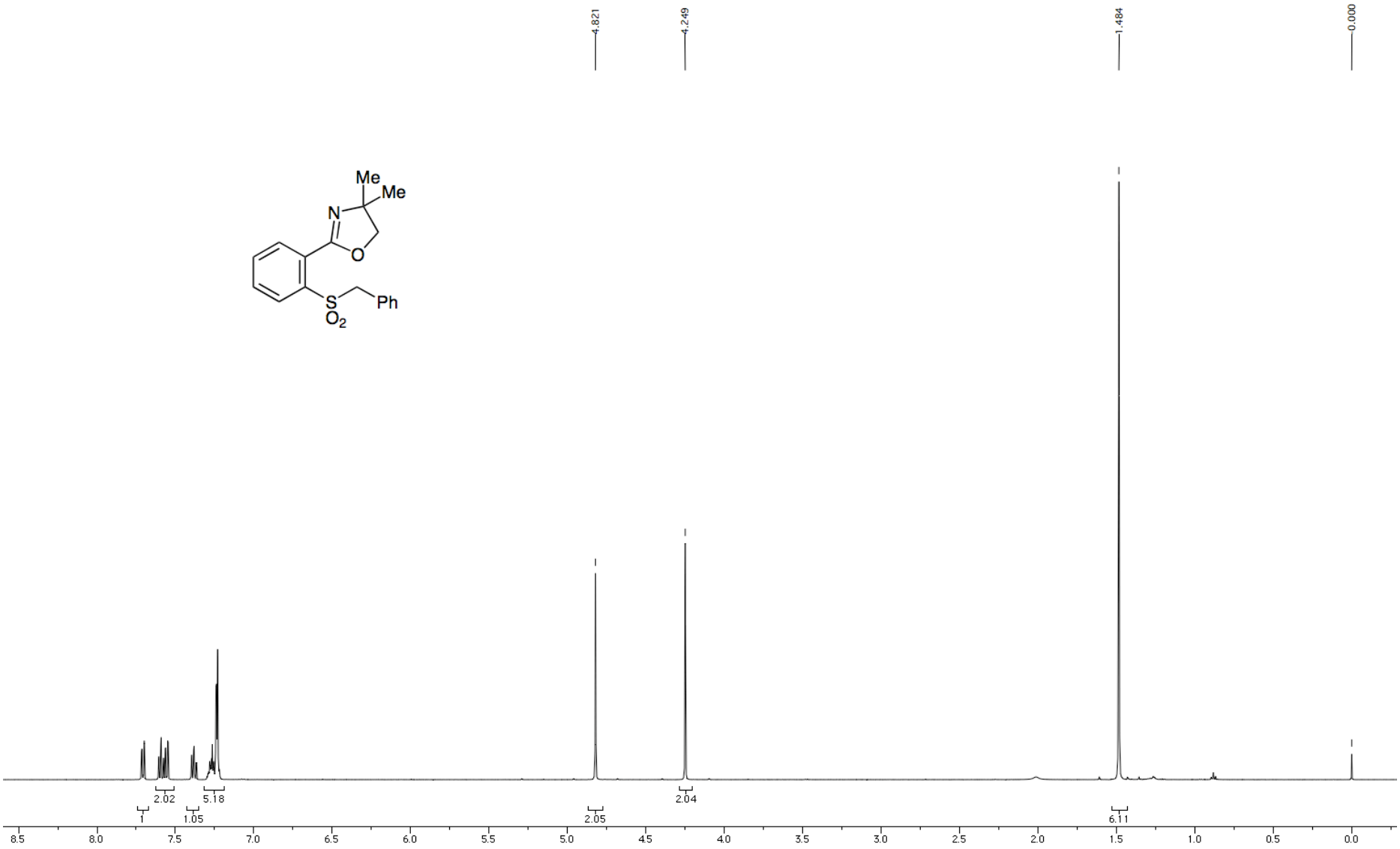
500 MHz ^{1}H NMR Spectrum of 2-Methyl-2-nitropropyl 2-(benzylsulfonyl)benzoate 19



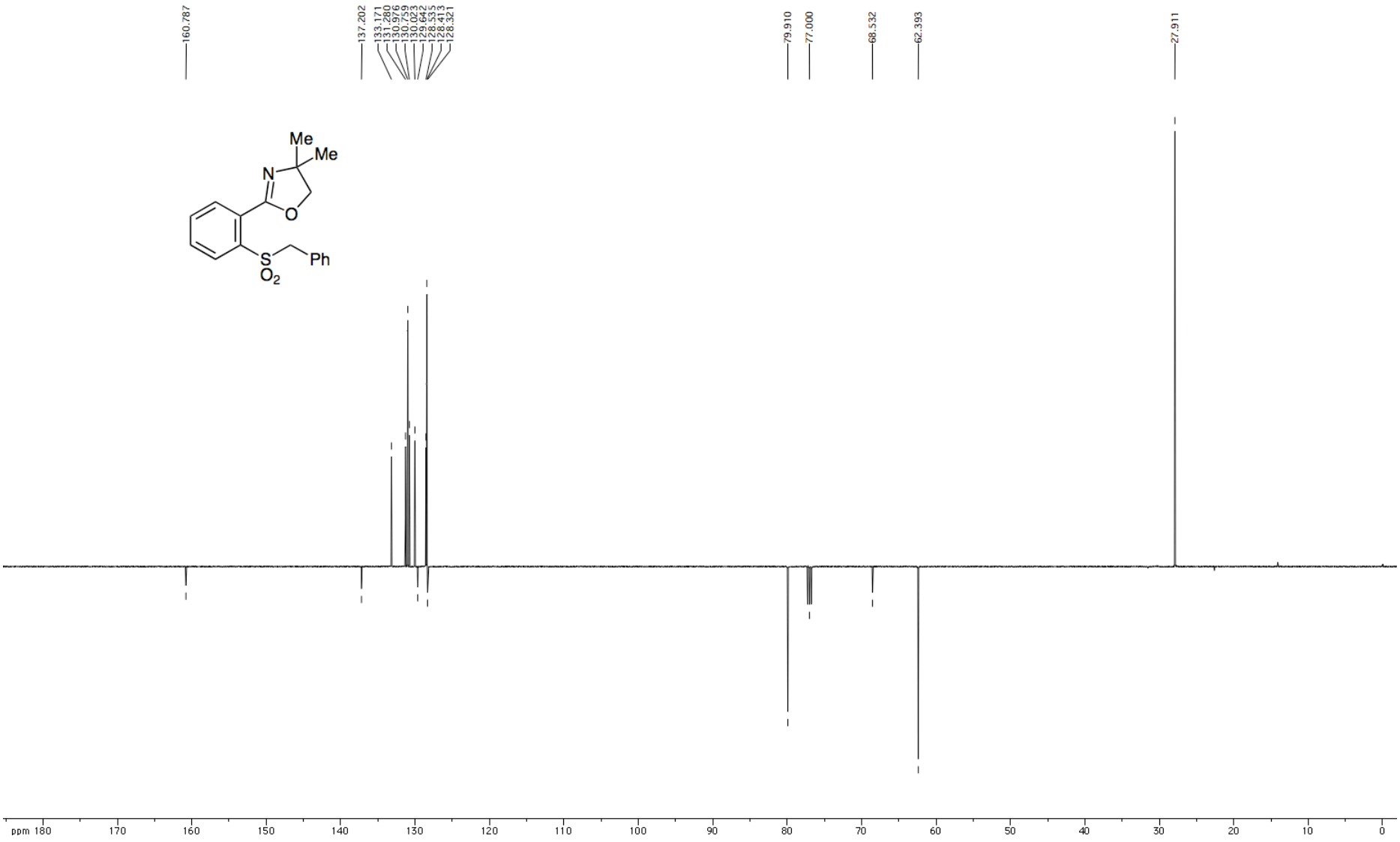
125 MHz DEPTQ ^{13}C NMR Spectrum of 2-Methyl-2-nitropropyl 2-(benzylsulfonyl)benzoate 19



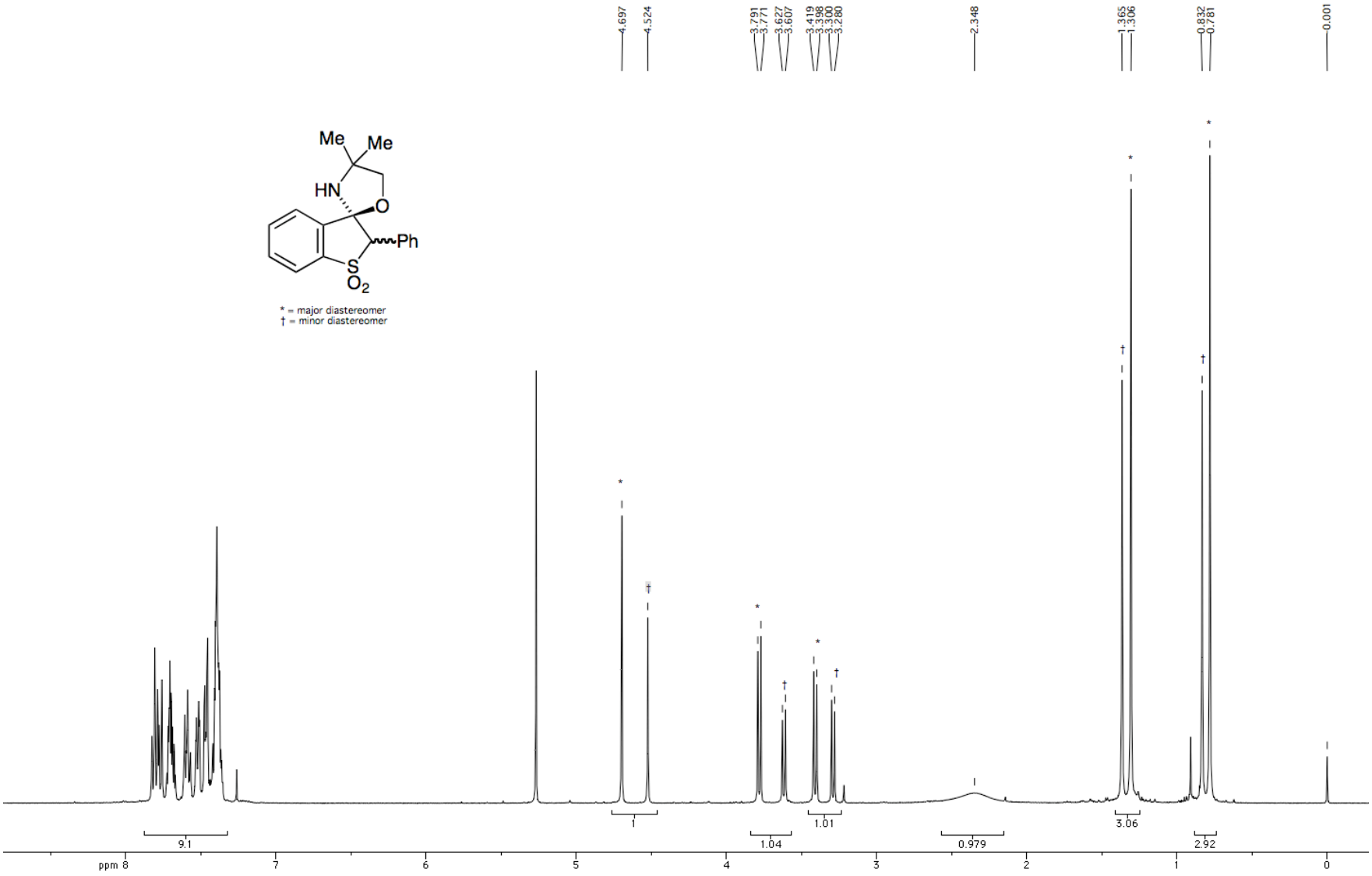
500 MHz ^{1}H NMR Spectrum of 2-(2-(Benzylsulfonyl)phenyl)-4,4-dimethyl-4,5-dihydrooxazole 18



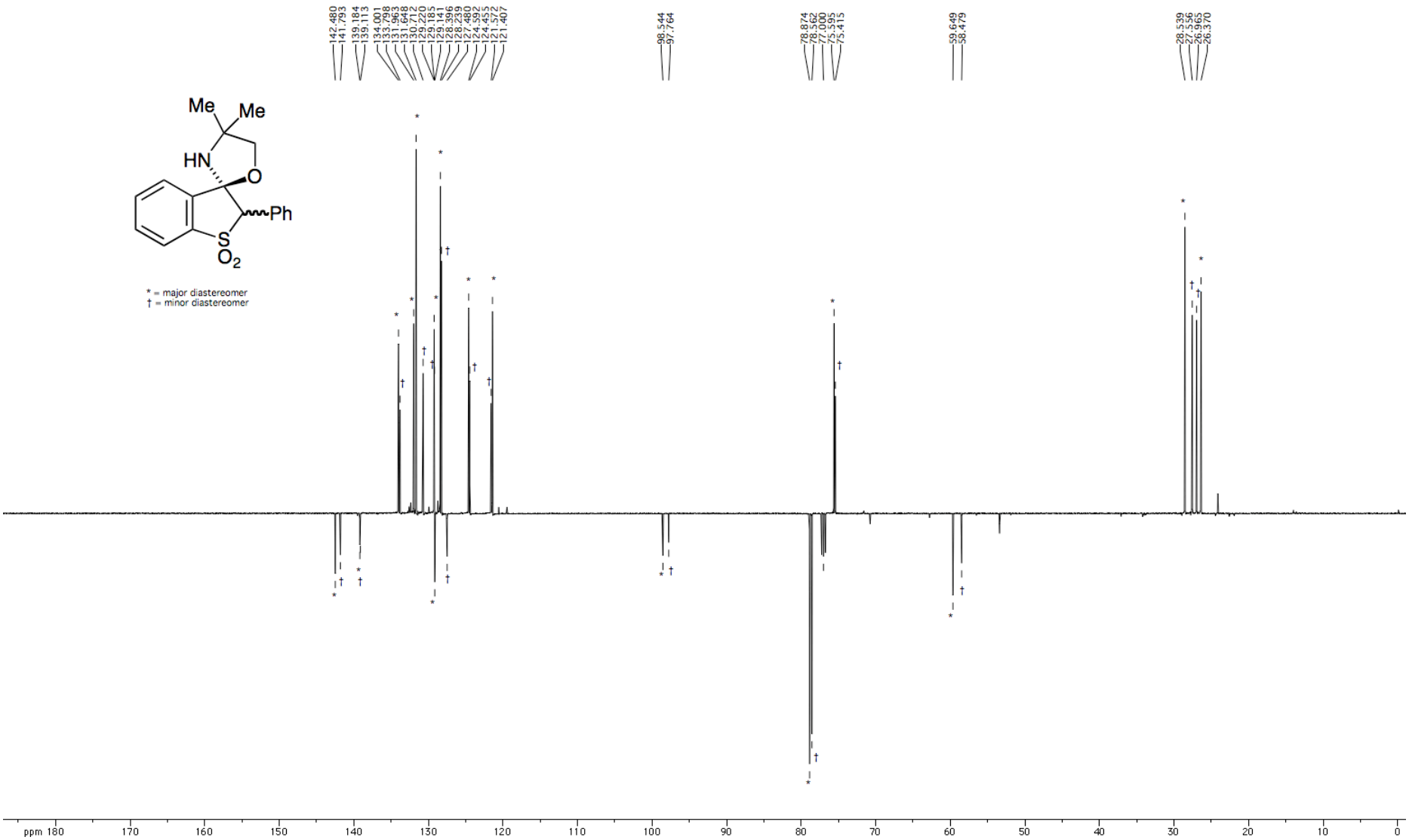
125 MHz DEPTQ ^{13}C NMR Spectrum of 2-(2-(Benzylsulfonyl)phenyl)-4,4-dimethyl-4,5-dihydrooxazole 18



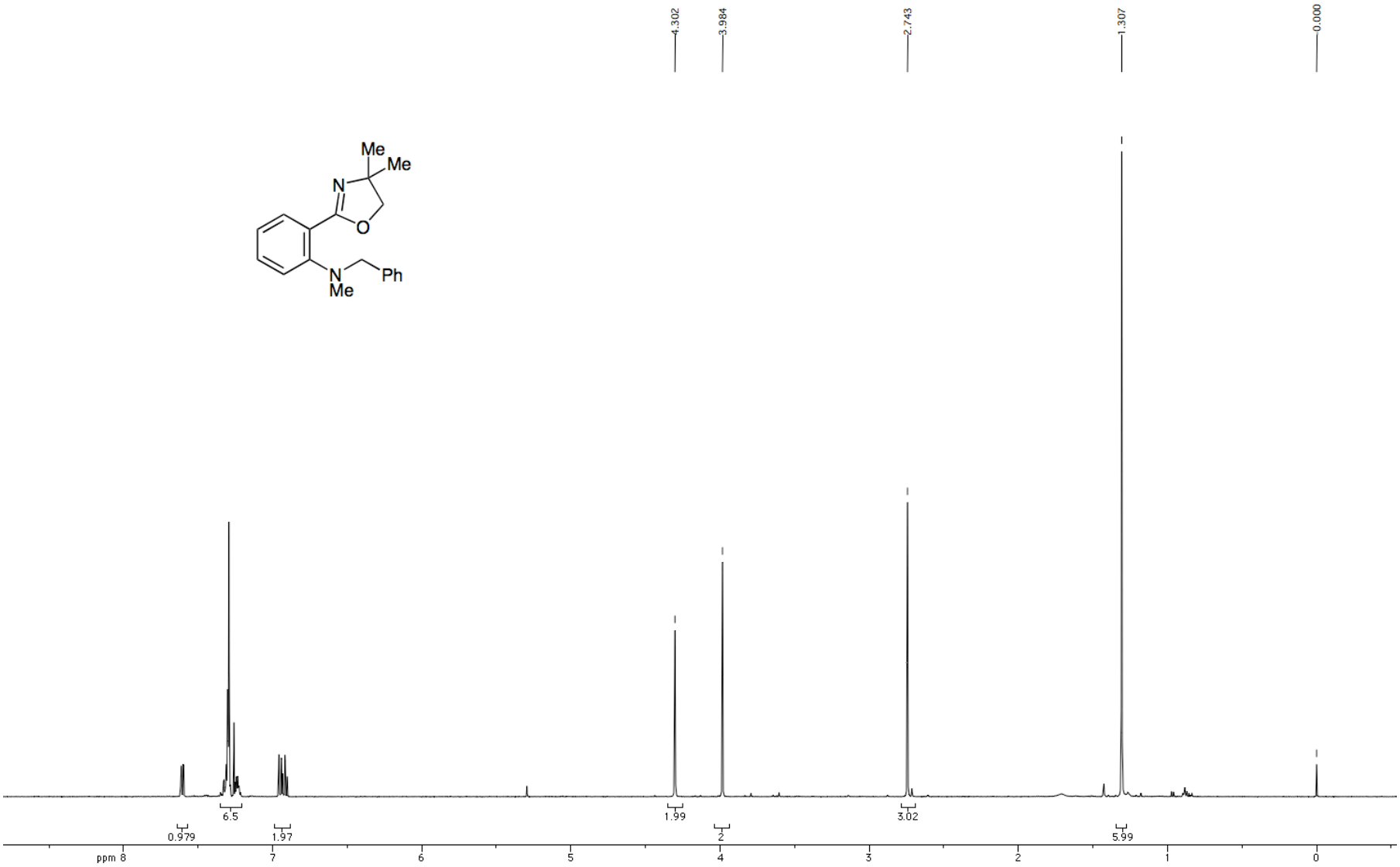
400 MHz ^{1}H NMR Spectrum of 4',4'-Dimethyl-2-phenyl-2*H*-spiro[benzo[*b*]thiophene-3,2'-oxazolidine] *S*,*S*-dioxide 20



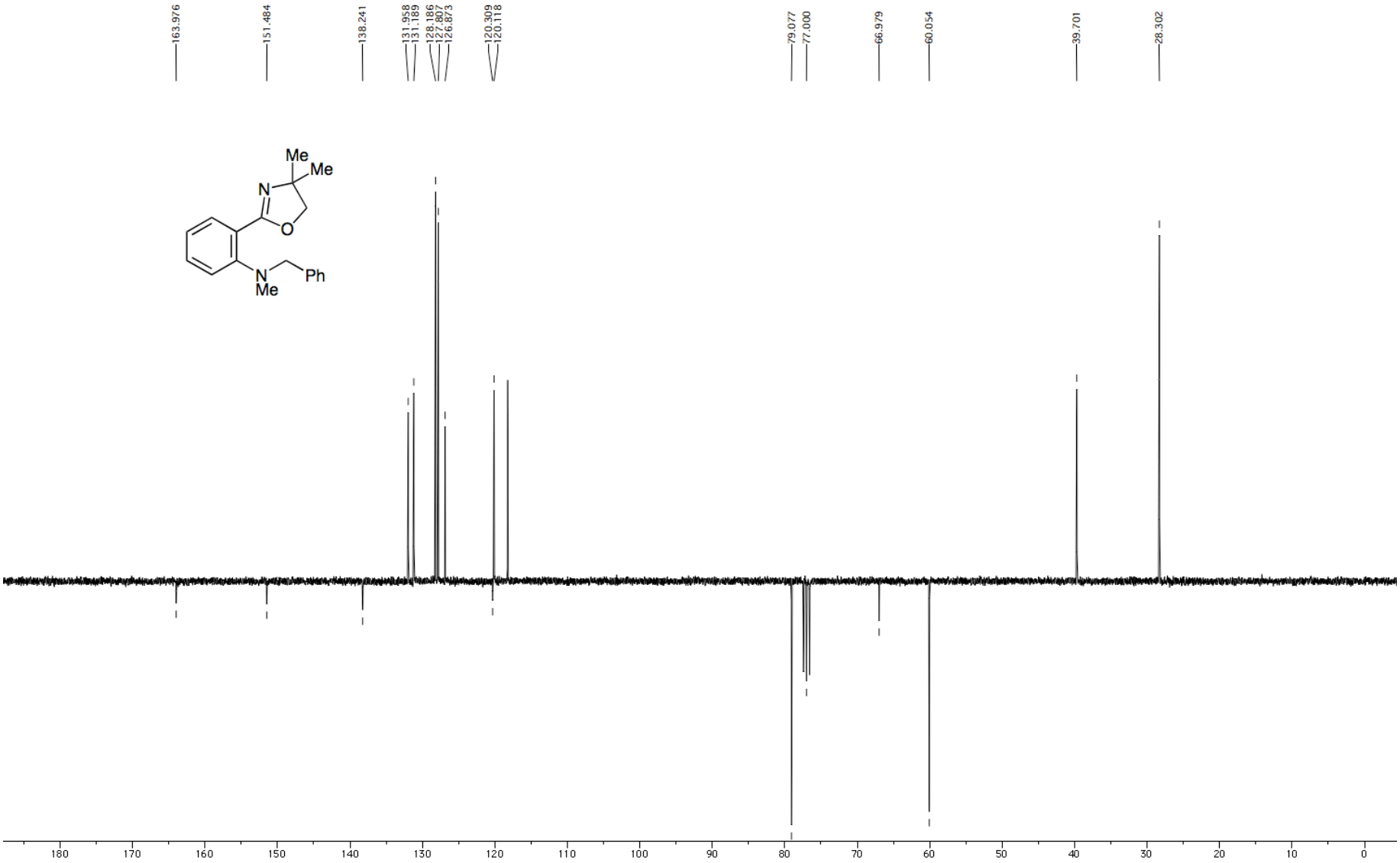
125 MHz DEPTQ ^{13}C NMR Spectrum of 4',4'-Dimethyl-2-phenyl-2*H*-spiro[benzo[*b*]thiophene-3,2'-oxazolidine] *S*,*S*-dioxide 20



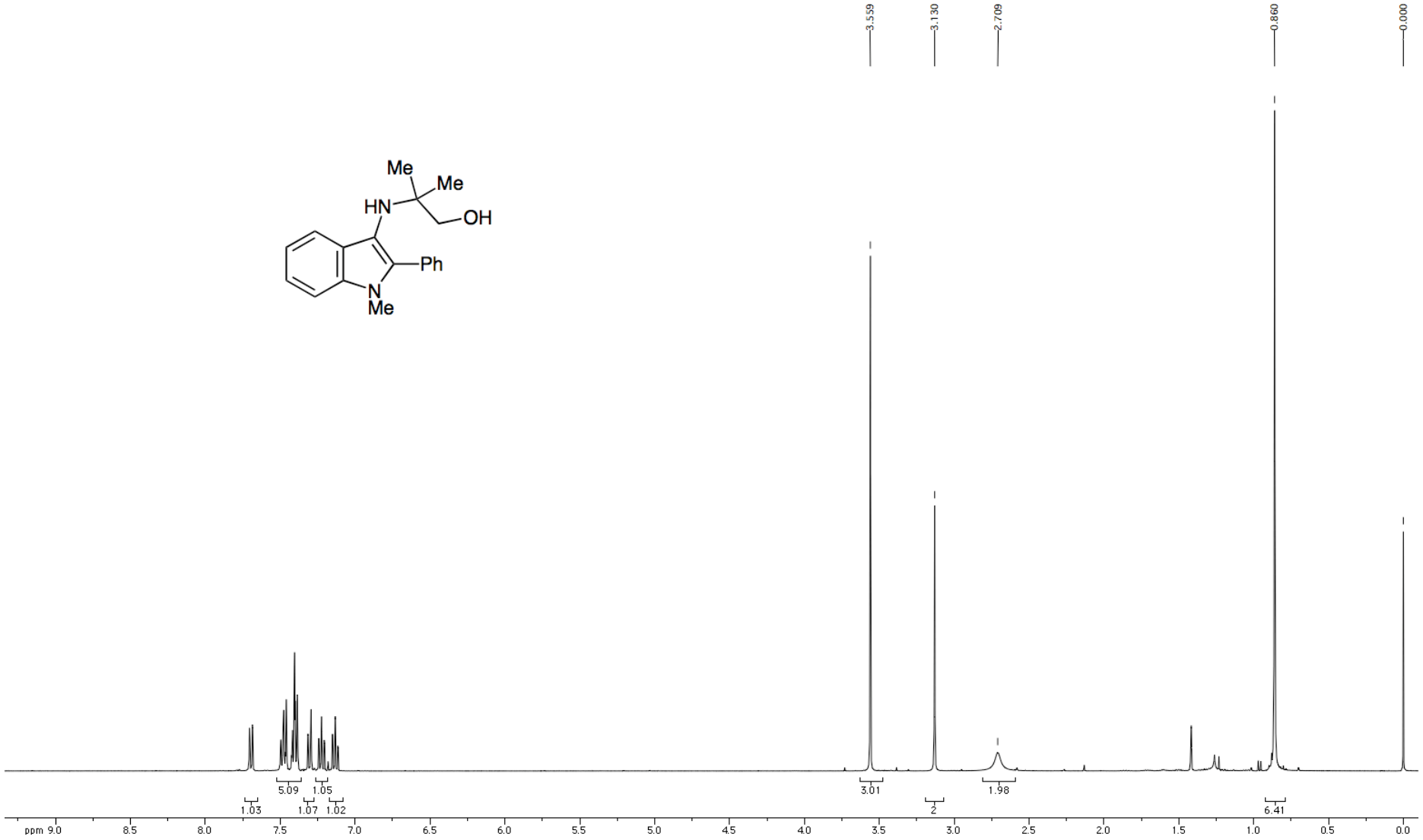
500 MHz ^{1}H NMR Spectrum of *N*-Benzyl-2-(4,4-dimethyl-4,5-dihydrooxazol-2-yl)-*N*-methylaniline 21



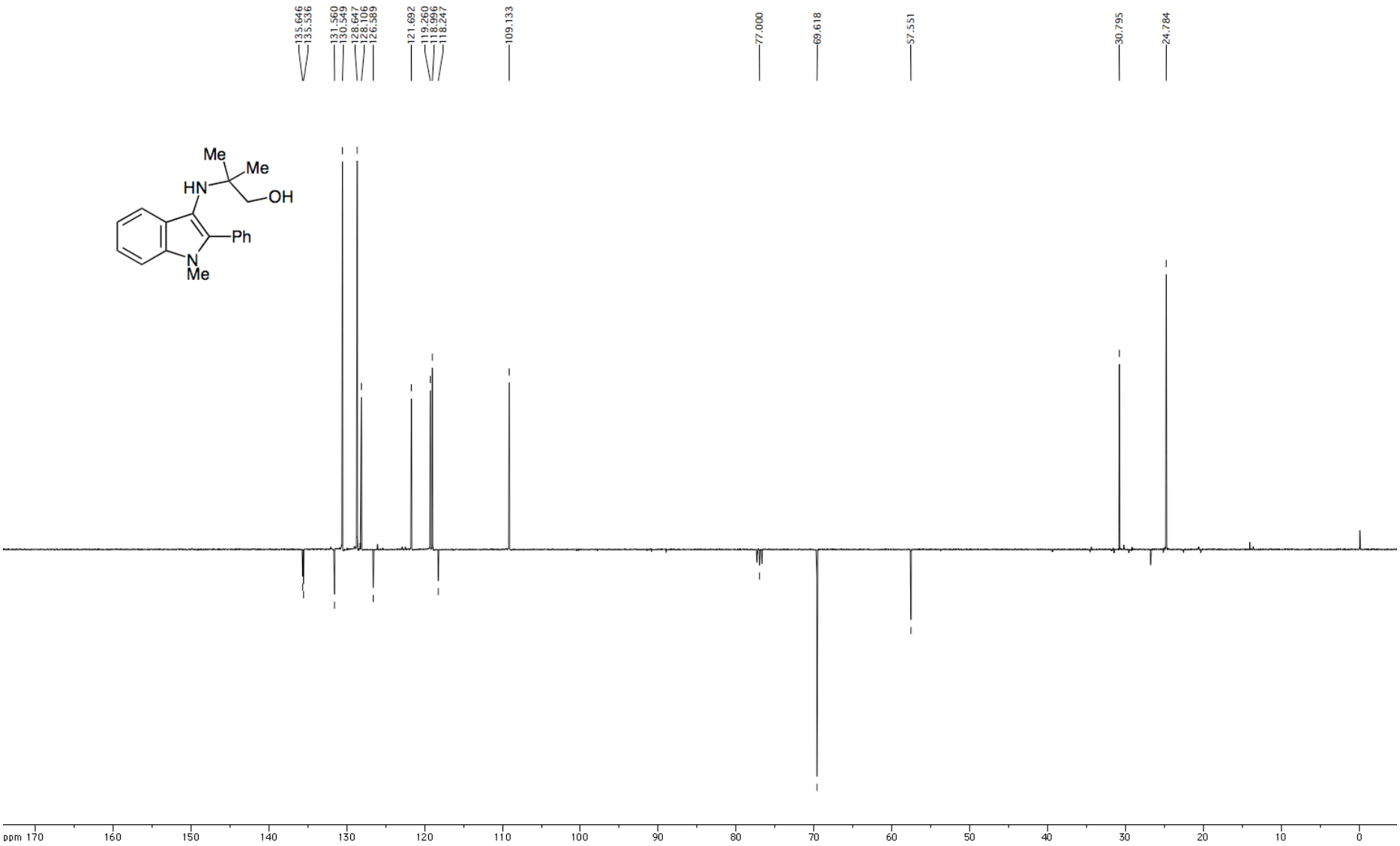
75 MHz DEPTQ ^{13}C NMR Spectrum of *N*-Benzyl-2-(4,4-dimethyl-4,5-dihydrooxazol-2-yl)-*N*-methylaniline 21



400 MHz ^{1}H NMR Spectrum of 2-Methyl-2-((1-methyl-2-phenyl-1*H*-indol-3-yl)amino)propan-1-ol 22



100 MHz DEPTQ ^{13}C NMR Spectrum of 2-Methyl-2-((1-methyl-2-phenyl-1*H*-indol-3-yl)amino)propan-1-ol 22



X-Ray structural details for Compound 16

CCDC No. 1540330

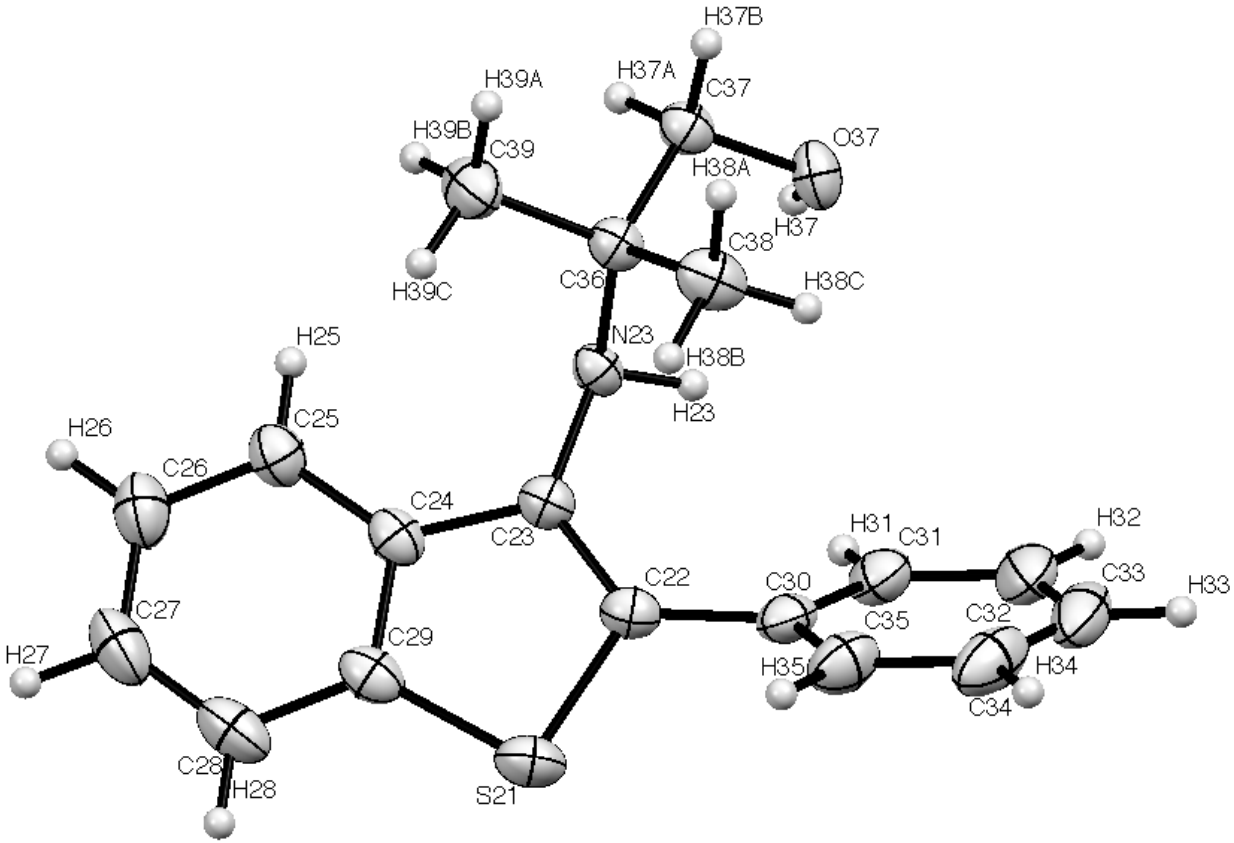
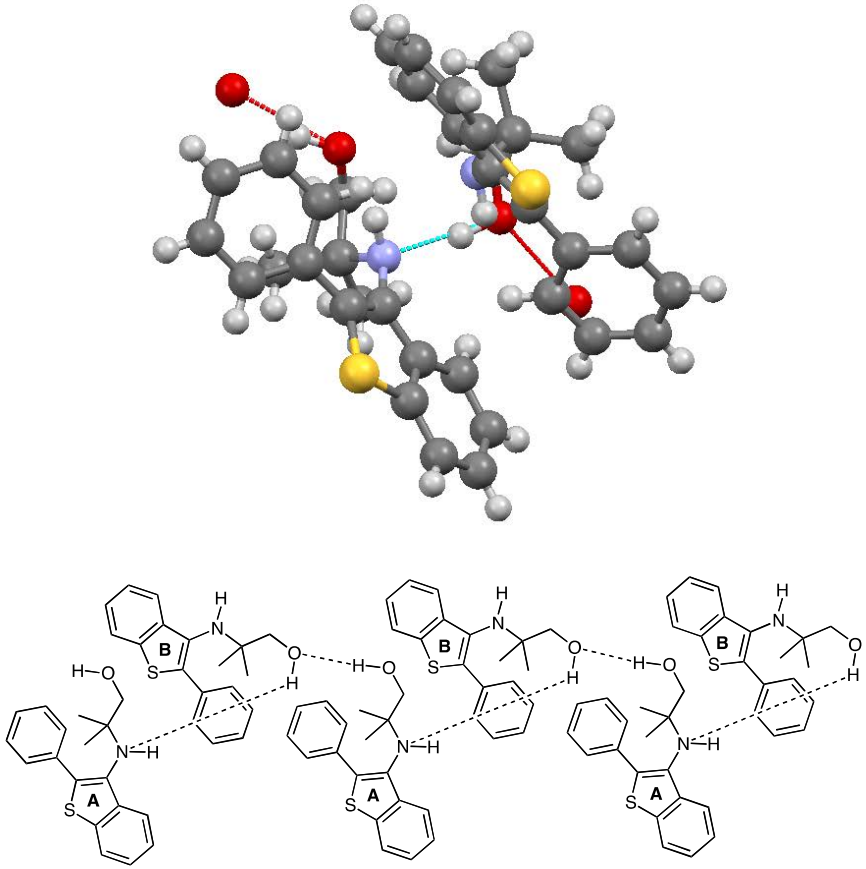


Figure 1. Molecular structure of one of the two distinct molecules in the unit cell of **16** (ORTEP diagram at 50% level)



Donor	H	Acceptor	D...A	D-H	H...A	D-H...A
O17 (A)	H17 (A)	O37 (B)	2.7504(17) Å	0.975(15) Å	1.811 (12) Å	161(2)°
O37 (B)	H37 (B)	N3 (A)	2.7836(16) Å	0.977(16) Å	1.819 (17) Å	169.1(16)°

Figure 2. Hydrogen bonding interaction between the two molecules of **16**